Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:45 PM GMT

PDB ID	:	1YAU
Title	:	Structure of Archeabacterial 20S proteasome- PA26 complex
Authors	:	Forster, A.; Masters, E.I.; Whitby, F.G.; Robinson, H.; Hill, C.P.
Deposited on	:	2004-12-17
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

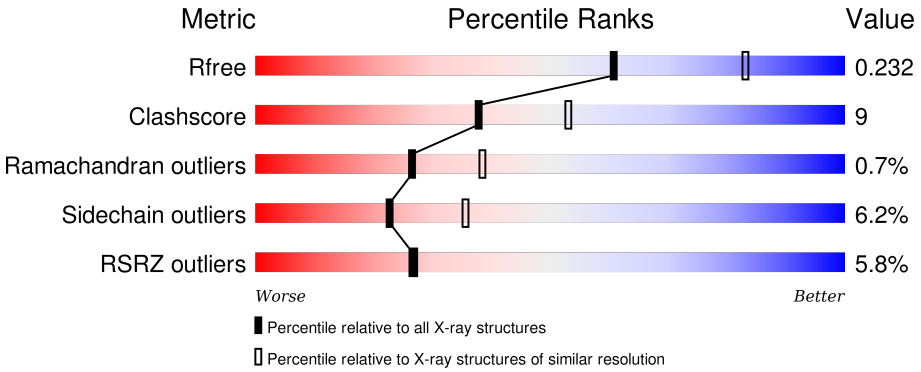
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	8% 68% 21% 6% 5%
1	B	233	7% 71% 20% • 5%
1	C	233	9% 76% 14% • 5%
1	D	233	8% 70% 21% • 5%
1	E	233	6% 69% 22% 5% 5%

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Mol	Chain	Length	Quality of chain
1	F	233	8% 76% 16% • 5%
1	G	233	9% 75% 17% • 5%
2	H	217	% 73% 17% • 6%
2	I	217	2% 73% 18% • 6%
2	J	217	% 76% 14% • 6%
2	K	217	3% 73% 18% • 6%
2	L	217	2% 70% 18% 5% • 6%
2	M	217	% 74% 18% • 6%
2	N	217	% 76% 14% • 6%
3	O	237	7% 75% 16% • 8%
3	P	237	5% 76% 15% • 8%
3	Q	237	7% 72% 19% 8%
3	R	237	7% 74% 17% 8%
3	S	237	5% 73% 18% 8%
3	T	237	5% 73% 18% • 8%
3	U	237	6% 77% 14% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	3007	-	-	X	-
4	SO4	H	3008	-	-	-	X
4	SO4	H	3015	-	-	-	X
4	SO4	I	3011	-	-	-	X
4	SO4	I	3016	-	-	-	X
4	SO4	I	3023	-	-	-	X
4	SO4	K	3013	-	-	-	X
4	SO4	K	3018	-	-	-	X
4	SO4	L	3014	-	-	-	X
4	SO4	M	3010	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	M	3025	-	-	-	X
4	SO4	N	3009	-	-	-	X
4	SO4	N	3022	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36610 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	B	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	C	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	D	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	E	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	F	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	G	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	TYR	ENGINEERED	UNP P25156
A	9	GLY	ASP	ENGINEERED	UNP P25156
B	8	GLY	TYR	ENGINEERED	UNP P25156
B	9	GLY	ASP	ENGINEERED	UNP P25156
C	8	GLY	TYR	ENGINEERED	UNP P25156
C	9	GLY	ASP	ENGINEERED	UNP P25156
D	8	GLY	TYR	ENGINEERED	UNP P25156
D	9	GLY	ASP	ENGINEERED	UNP P25156
E	8	GLY	TYR	ENGINEERED	UNP P25156
E	9	GLY	ASP	ENGINEERED	UNP P25156
F	8	GLY	TYR	ENGINEERED	UNP P25156
F	9	GLY	ASP	ENGINEERED	UNP P25156
G	8	GLY	TYR	ENGINEERED	UNP P25156
G	9	GLY	ASP	ENGINEERED	UNP P25156

- Molecule 2 is a protein called Proteasome beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			
2	I	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			
2	J	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			
2	K	203	Total	C	N	O	S	0	1	0
			1569	994	265	299	11			
2	L	203	Total	C	N	O	S	0	1	0
			1569	994	265	299	11			
2	M	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			
2	N	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	204	HIS	-	EXPRESSION TAG	UNP P28061
H	205	HIS	-	EXPRESSION TAG	UNP P28061
H	206	HIS	-	EXPRESSION TAG	UNP P28061
H	207	HIS	-	EXPRESSION TAG	UNP P28061
H	208	HIS	-	EXPRESSION TAG	UNP P28061
H	209	HIS	-	EXPRESSION TAG	UNP P28061
I	204	HIS	-	EXPRESSION TAG	UNP P28061
I	205	HIS	-	EXPRESSION TAG	UNP P28061
I	206	HIS	-	EXPRESSION TAG	UNP P28061
I	207	HIS	-	EXPRESSION TAG	UNP P28061
I	208	HIS	-	EXPRESSION TAG	UNP P28061
I	209	HIS	-	EXPRESSION TAG	UNP P28061
J	204	HIS	-	EXPRESSION TAG	UNP P28061
J	205	HIS	-	EXPRESSION TAG	UNP P28061
J	206	HIS	-	EXPRESSION TAG	UNP P28061
J	207	HIS	-	EXPRESSION TAG	UNP P28061
J	208	HIS	-	EXPRESSION TAG	UNP P28061
J	209	HIS	-	EXPRESSION TAG	UNP P28061
K	204	HIS	-	EXPRESSION TAG	UNP P28061
K	205	HIS	-	EXPRESSION TAG	UNP P28061
K	206	HIS	-	EXPRESSION TAG	UNP P28061
K	207	HIS	-	EXPRESSION TAG	UNP P28061
K	208	HIS	-	EXPRESSION TAG	UNP P28061
K	209	HIS	-	EXPRESSION TAG	UNP P28061

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Chain	Residue	Modelled	Actual	Comment	Reference
L	204	HIS	-	EXPRESSION TAG	UNP P28061
L	205	HIS	-	EXPRESSION TAG	UNP P28061
L	206	HIS	-	EXPRESSION TAG	UNP P28061
L	207	HIS	-	EXPRESSION TAG	UNP P28061
L	208	HIS	-	EXPRESSION TAG	UNP P28061
L	209	HIS	-	EXPRESSION TAG	UNP P28061
M	204	HIS	-	EXPRESSION TAG	UNP P28061
M	205	HIS	-	EXPRESSION TAG	UNP P28061
M	206	HIS	-	EXPRESSION TAG	UNP P28061
M	207	HIS	-	EXPRESSION TAG	UNP P28061
M	208	HIS	-	EXPRESSION TAG	UNP P28061
M	209	HIS	-	EXPRESSION TAG	UNP P28061
N	204	HIS	-	EXPRESSION TAG	UNP P28061
N	205	HIS	-	EXPRESSION TAG	UNP P28061
N	206	HIS	-	EXPRESSION TAG	UNP P28061
N	207	HIS	-	EXPRESSION TAG	UNP P28061
N	208	HIS	-	EXPRESSION TAG	UNP P28061
N	209	HIS	-	EXPRESSION TAG	UNP P28061

- Molecule 3 is a protein called proteasome activator protein PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	P	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	Q	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	R	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	S	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	T	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	U	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	MET	-	INITIATING METHIONINE	GB 5757773
O	-4	HIS	-	EXPRESSION TAG	GB 5757773

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-3	HIS	-	EXPRESSION TAG	GB 5757773
O	-2	HIS	-	EXPRESSION TAG	GB 5757773
O	-1	HIS	-	EXPRESSION TAG	GB 5757773
O	0	HIS	-	EXPRESSION TAG	GB 5757773
O	1	HIS	-	EXPRESSION TAG	GB 5757773
O	49	VAL	THR	VARIANT	GB 5757773
P	-5	MET	-	INITIATING METHIONINE	GB 5757773
P	-4	HIS	-	EXPRESSION TAG	GB 5757773
P	-3	HIS	-	EXPRESSION TAG	GB 5757773
P	-2	HIS	-	EXPRESSION TAG	GB 5757773
P	-1	HIS	-	EXPRESSION TAG	GB 5757773
P	0	HIS	-	EXPRESSION TAG	GB 5757773
P	1	HIS	-	EXPRESSION TAG	GB 5757773
P	49	VAL	THR	VARIANT	GB 5757773
Q	-5	MET	-	INITIATING METHIONINE	GB 5757773
Q	-4	HIS	-	EXPRESSION TAG	GB 5757773
Q	-3	HIS	-	EXPRESSION TAG	GB 5757773
Q	-2	HIS	-	EXPRESSION TAG	GB 5757773
Q	-1	HIS	-	EXPRESSION TAG	GB 5757773
Q	0	HIS	-	EXPRESSION TAG	GB 5757773
Q	1	HIS	-	EXPRESSION TAG	GB 5757773
Q	49	VAL	THR	VARIANT	GB 5757773
R	-5	MET	-	INITIATING METHIONINE	GB 5757773
R	-4	HIS	-	EXPRESSION TAG	GB 5757773
R	-3	HIS	-	EXPRESSION TAG	GB 5757773
R	-2	HIS	-	EXPRESSION TAG	GB 5757773
R	-1	HIS	-	EXPRESSION TAG	GB 5757773
R	0	HIS	-	EXPRESSION TAG	GB 5757773
R	1	HIS	-	EXPRESSION TAG	GB 5757773
R	49	VAL	THR	VARIANT	GB 5757773
S	-5	MET	-	INITIATING METHIONINE	GB 5757773
S	-4	HIS	-	EXPRESSION TAG	GB 5757773
S	-3	HIS	-	EXPRESSION TAG	GB 5757773
S	-2	HIS	-	EXPRESSION TAG	GB 5757773
S	-1	HIS	-	EXPRESSION TAG	GB 5757773
S	0	HIS	-	EXPRESSION TAG	GB 5757773
S	1	HIS	-	EXPRESSION TAG	GB 5757773
S	49	VAL	THR	VARIANT	GB 5757773
T	-5	MET	-	INITIATING METHIONINE	GB 5757773
T	-4	HIS	-	EXPRESSION TAG	GB 5757773
T	-3	HIS	-	EXPRESSION TAG	GB 5757773
T	-2	HIS	-	EXPRESSION TAG	GB 5757773

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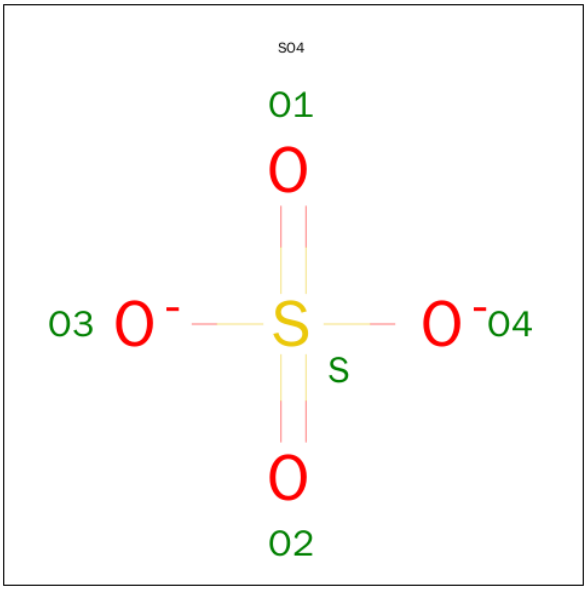
Chain	Residue	Modelled	Actual	Comment	Reference
T	-1	HIS	-	EXPRESSION TAG	GB 5757773
T	0	HIS	-	EXPRESSION TAG	GB 5757773
T	1	HIS	-	EXPRESSION TAG	GB 5757773
T	49	VAL	THR	VARIANT	GB 5757773
U	-5	MET	-	INITIATING METHIONINE	GB 5757773
U	-4	HIS	-	EXPRESSION TAG	GB 5757773
U	-3	HIS	-	EXPRESSION TAG	GB 5757773
U	-2	HIS	-	EXPRESSION TAG	GB 5757773
U	-1	HIS	-	EXPRESSION TAG	GB 5757773
U	0	HIS	-	EXPRESSION TAG	GB 5757773
U	1	HIS	-	EXPRESSION TAG	GB 5757773
U	49	VAL	THR	VARIANT	GB 5757773

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

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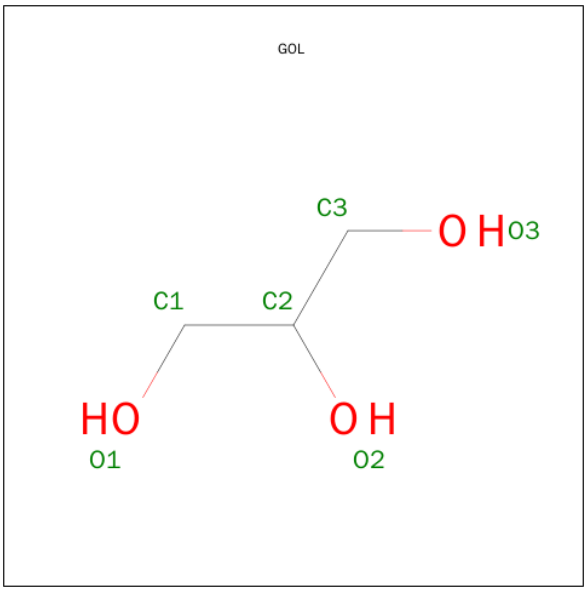
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O 6 3 3	0	0
5	M	1	Total C O 6 3 3	0	0
5	N	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	67	Total O 67 67	0	0
6	B	58	Total O 58 58	0	0
6	C	69	Total O 69 69	0	0
6	D	49	Total O 49 49	0	0
6	E	67	Total O 67 67	0	0

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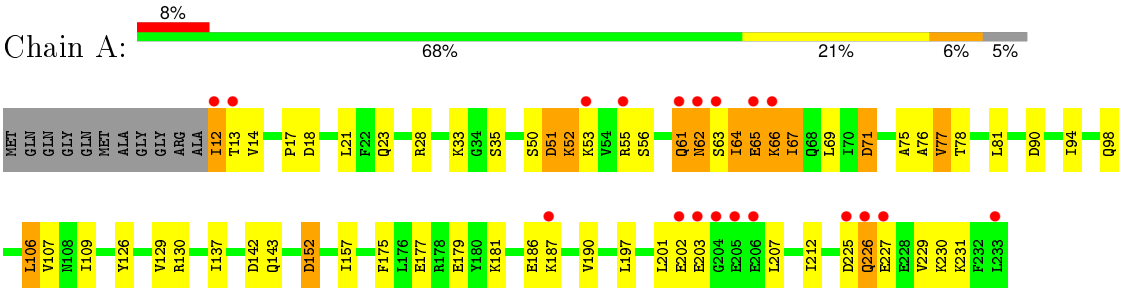
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	61	Total O 61 61	0	0
6	G	51	Total O 51 51	0	0
6	H	93	Total O 93 93	0	0
6	I	100	Total O 100 100	0	0
6	J	94	Total O 94 94	0	0
6	K	85	Total O 85 85	0	0
6	L	93	Total O 93 93	0	0
6	M	100	Total O 100 100	0	0
6	N	107	Total O 107 107	0	0
6	O	52	Total O 52 52	0	0
6	P	47	Total O 47 47	0	0
6	Q	47	Total O 47 47	0	0
6	R	69	Total O 69 69	0	0
6	S	90	Total O 90 90	0	0
6	T	97	Total O 97 97	0	0
6	U	75	Total O 75 75	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

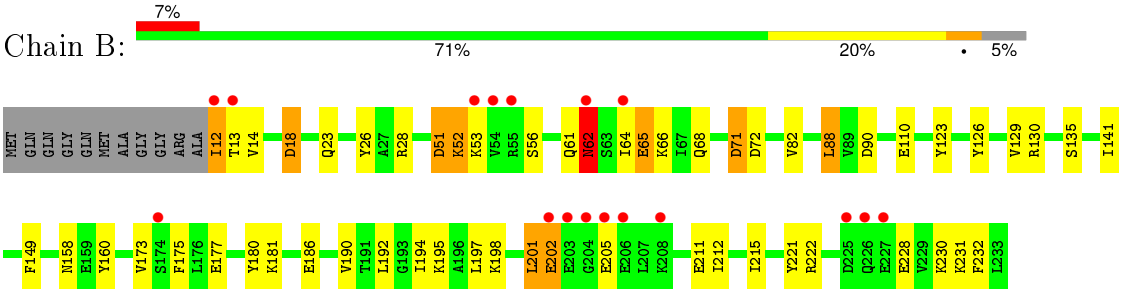
- Molecule 1: Proteasome alpha subunit

Chain A:



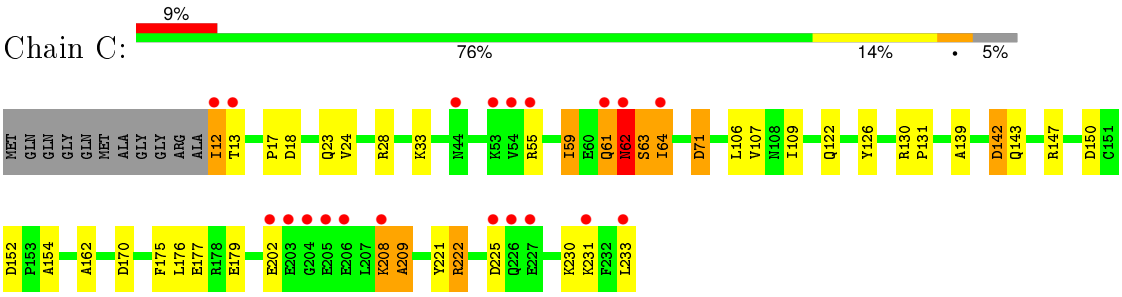
- Molecule 1: Proteasome alpha subunit

Chain B:



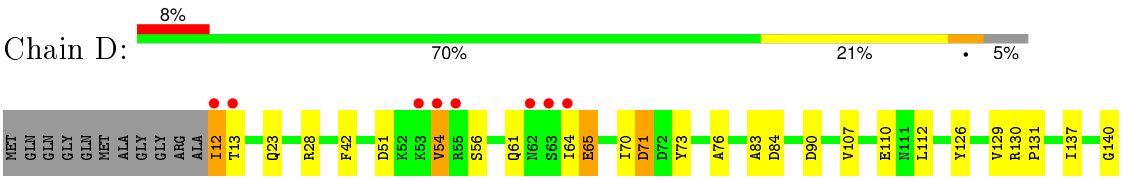
- Molecule 1: Proteasome alpha subunit

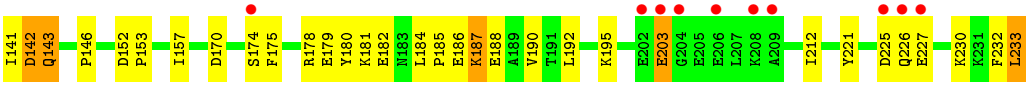
Chain C:



- Molecule 1: Proteasome alpha subunit

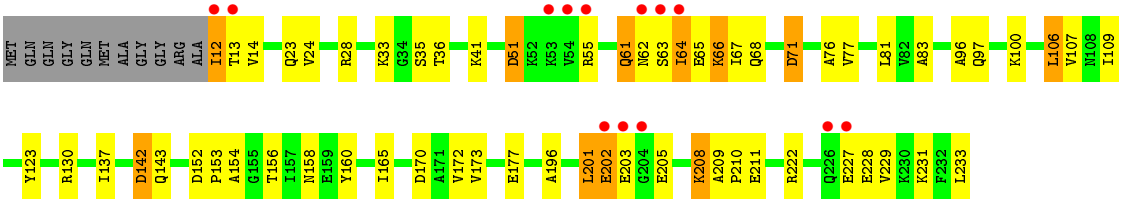
Chain D:





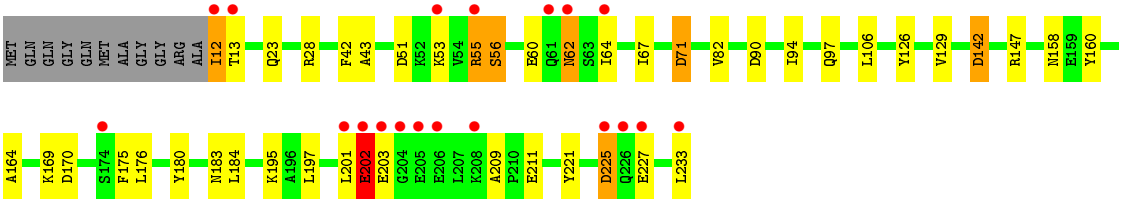
- Molecule 1: Proteasome alpha subunit

Chain E:



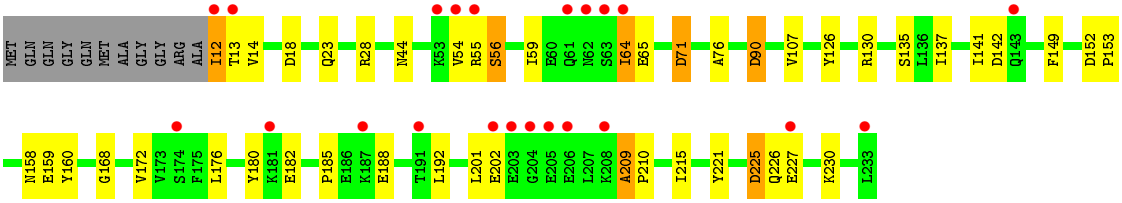
- Molecule 1: Proteasome alpha subunit

Chain F:



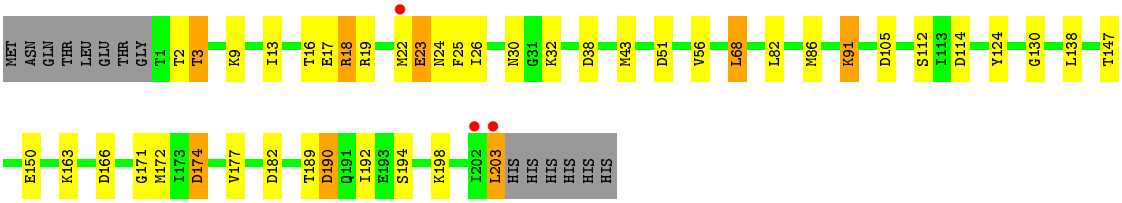
- Molecule 1: Proteasome alpha subunit

Chain G:



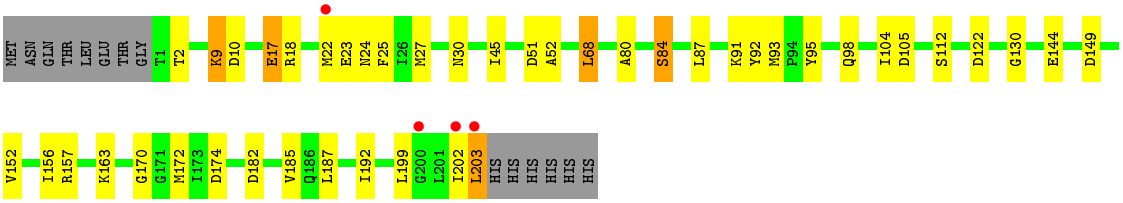
- Molecule 2: Proteasome beta subunit

Chain H:



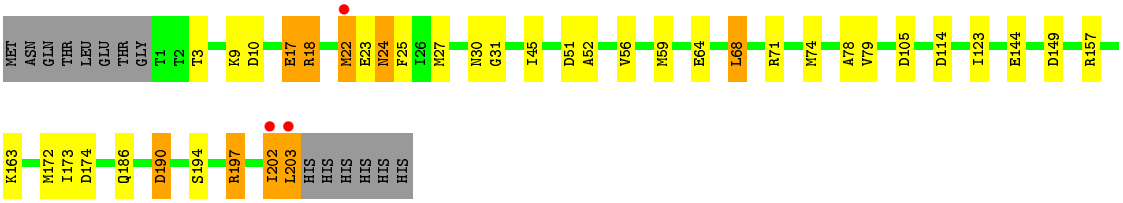
- Molecule 2: Proteasome beta subunit

Chain I:



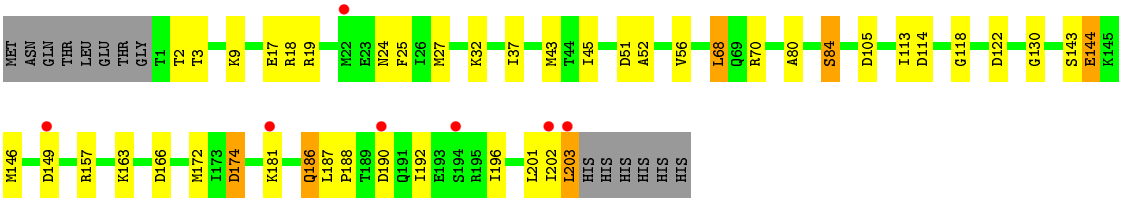
• Molecule 2: Proteasome beta subunit

Chain J:



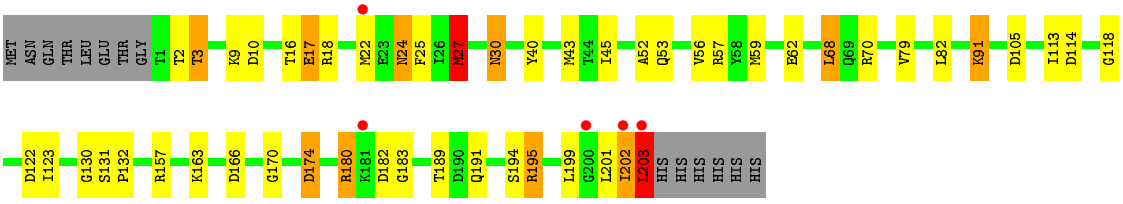
• Molecule 2: Proteasome beta subunit

Chain K:



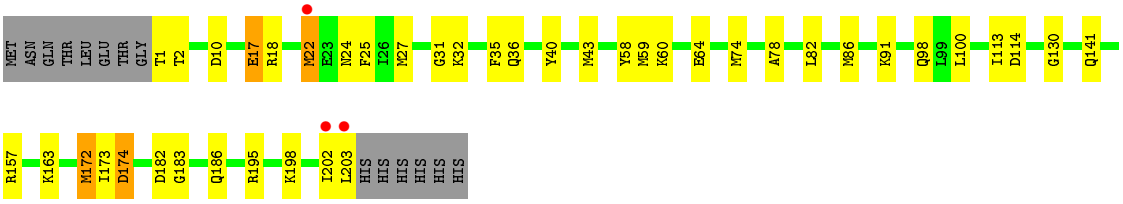
• Molecule 2: Proteasome beta subunit

Chain L:



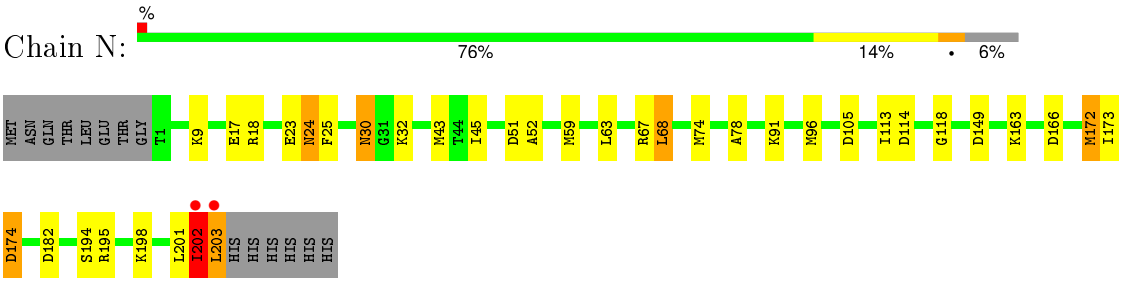
• Molecule 2: Proteasome beta subunit

Chain M:



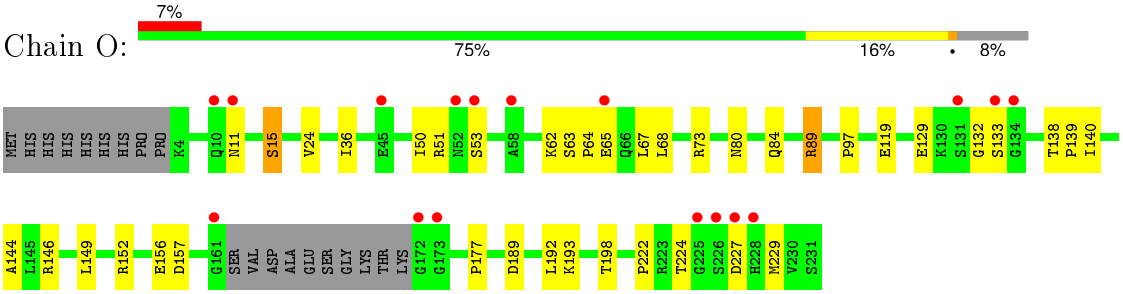
• Molecule 2: Proteasome beta subunit

Chain N:



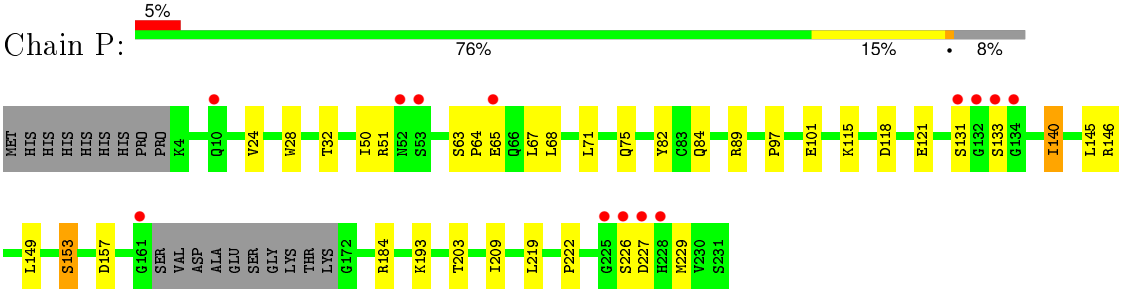
• Molecule 3: proteasome activator protein PA26

Chain O:



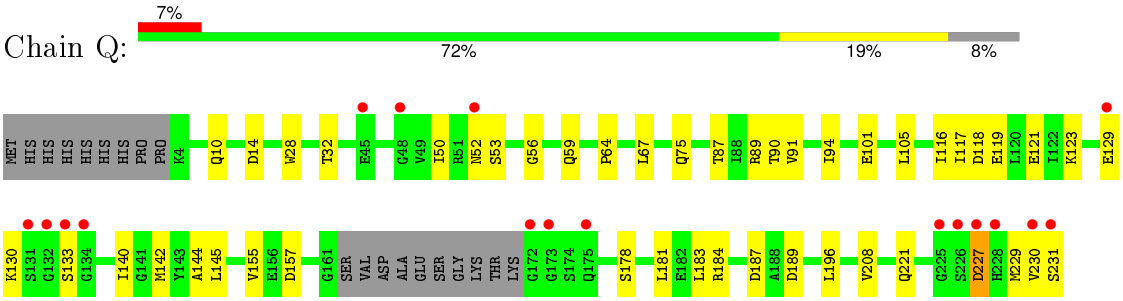
• Molecule 3: proteasome activator protein PA26

Chain P:



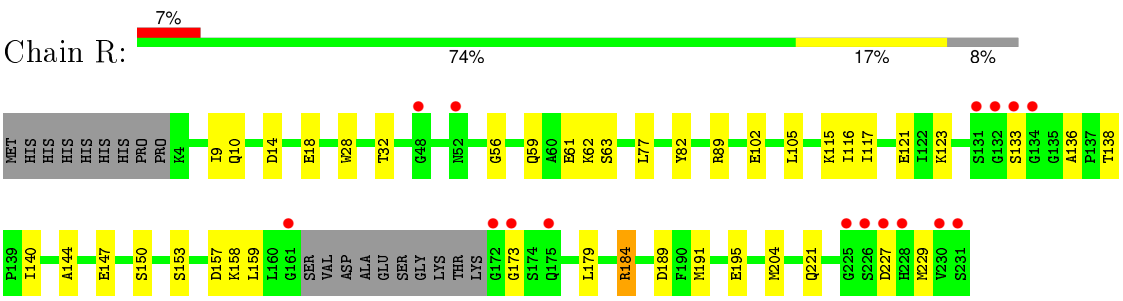
• Molecule 3: proteasome activator protein PA26

Chain Q:



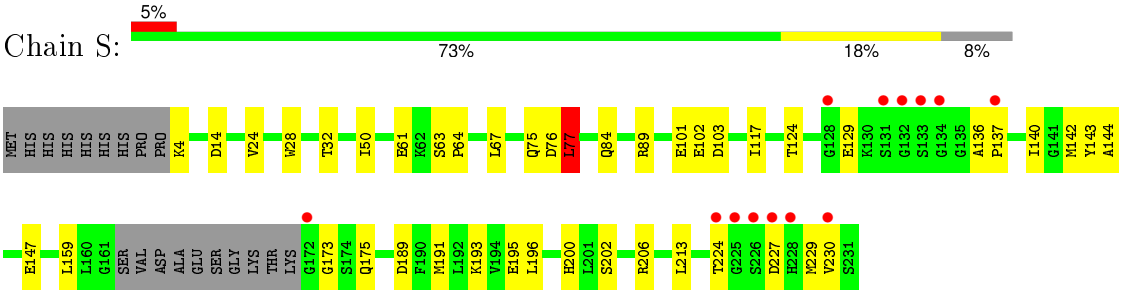
• Molecule 3: proteasome activator protein PA26

Chain R:



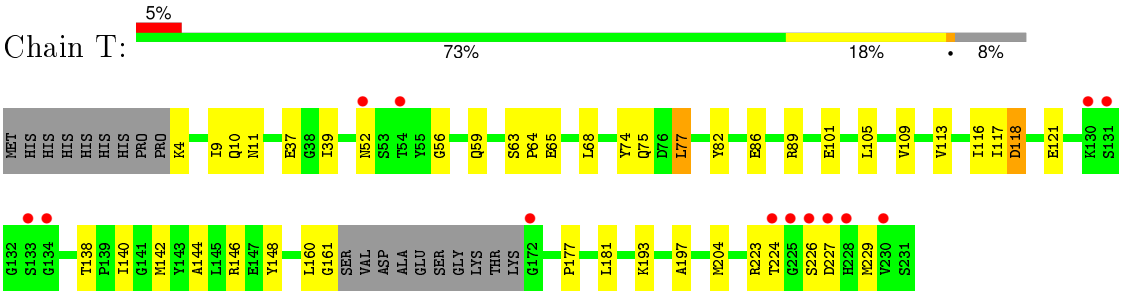
• Molecule 3: proteasome activator protein PA26

Chain S:



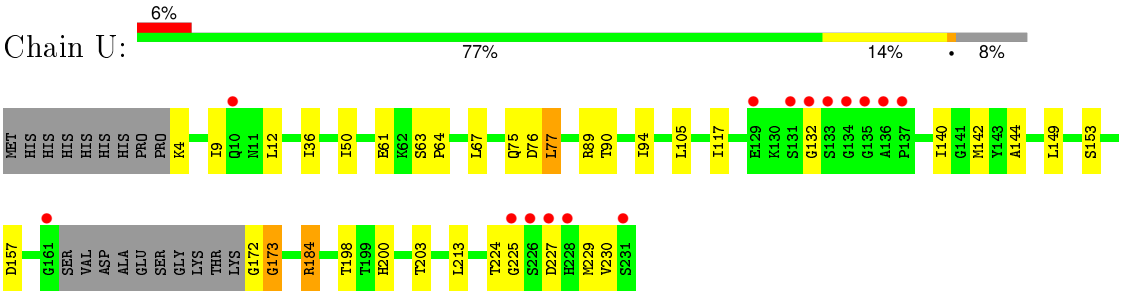
• Molecule 3: proteasome activator protein PA26

Chain T:



• Molecule 3: proteasome activator protein PA26

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	255.22Å 126.91Å 181.03Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 8.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (8.00-2.40) 99.8 (8.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.180 , 0.233 0.180 , 0.232	Depositor DCC
R_{free} test set	1069 reflections (0.49%)	DCC
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.51 , 74.4	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 218327 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	36610	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.80	0/1751	0.88	3/2359 (0.1%)
1	B	0.83	0/1751	0.91	5/2359 (0.2%)
1	C	0.80	0/1751	0.87	6/2359 (0.3%)
1	D	0.77	0/1751	0.91	6/2359 (0.3%)
1	E	0.81	0/1751	0.88	5/2359 (0.2%)
1	F	0.74	0/1751	0.85	4/2359 (0.2%)
1	G	0.78	0/1751	0.89	3/2359 (0.1%)
2	H	0.85	0/1597	0.94	6/2157 (0.3%)
2	I	0.84	0/1597	0.95	5/2157 (0.2%)
2	J	0.88	0/1597	0.93	5/2157 (0.2%)
2	K	0.82	0/1589	1.00	10/2147 (0.5%)
2	L	0.84	0/1589	0.97	8/2147 (0.4%)
2	M	0.87	0/1597	0.96	4/2157 (0.2%)
2	N	0.82	0/1597	0.95	6/2157 (0.3%)
3	O	0.66	0/1702	0.79	2/2299 (0.1%)
3	P	0.64	0/1702	0.78	2/2299 (0.1%)
3	Q	0.66	0/1702	0.79	3/2299 (0.1%)
3	R	0.71	0/1702	0.81	3/2299 (0.1%)
3	S	0.75	0/1702	0.84	5/2299 (0.2%)
3	T	0.77	0/1702	0.83	3/2299 (0.1%)
3	U	0.76	0/1702	0.82	2/2299 (0.1%)
All	All	0.78	0/35334	0.88	96/47685 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	174	ASP	CB-CG-OD2	10.79	128.01	118.30
2	N	203	LEU	CA-CB-CG	9.32	136.73	115.30
3	S	227	ASP	CB-CG-OD2	8.09	125.58	118.30
1	A	142	ASP	CB-CG-OD2	7.99	125.49	118.30
1	F	142	ASP	CB-CG-OD2	7.72	125.25	118.30
3	U	227	ASP	CB-CG-OD2	7.68	125.21	118.30
3	P	227	ASP	CB-CG-OD2	7.61	125.15	118.30
1	D	71	ASP	CB-CG-OD2	7.52	125.07	118.30
1	G	71	ASP	CB-CG-OD2	7.46	125.01	118.30
1	B	71	ASP	CB-CG-OD2	7.41	124.97	118.30
1	D	142	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	71	ASP	CB-CG-OD2	7.10	124.69	118.30
3	O	227	ASP	CB-CG-OD2	7.07	124.66	118.30
1	E	71	ASP	CB-CG-OD2	6.91	124.52	118.30
2	L	122	ASP	CB-CG-OD2	6.87	124.48	118.30
2	H	38	ASP	CB-CG-OD2	6.87	124.48	118.30
2	N	149	ASP	CB-CG-OD2	6.84	124.45	118.30
2	K	19	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	170	ASP	CB-CG-OD2	6.64	124.28	118.30
3	T	118	ASP	CB-CG-OD2	6.62	124.26	118.30
2	K	174	ASP	CB-CG-OD1	-6.60	112.36	118.30
2	L	166	ASP	CB-CG-OD2	6.55	124.20	118.30
3	T	227	ASP	CB-CG-OD2	6.52	124.17	118.30
1	E	142	ASP	CB-CG-OD2	6.45	124.11	118.30
2	K	19	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	C	225	ASP	CB-CG-OD2	6.37	124.03	118.30
3	P	157	ASP	CB-CG-OD2	6.34	124.01	118.30
3	U	157	ASP	CB-CG-OD2	6.28	123.95	118.30
2	H	182	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	18	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	71	ASP	CB-CG-OD2	6.18	123.86	118.30
2	I	149	ASP	CB-CG-OD2	6.18	123.86	118.30
2	I	122	ASP	CB-CG-OD2	6.14	123.82	118.30
3	S	76	ASP	CB-CG-OD2	6.13	123.82	118.30
2	J	114	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	170	ASP	CB-CG-OD2	6.10	123.79	118.30
1	F	71	ASP	CB-CG-OD2	6.06	123.76	118.30
2	K	114	ASP	CB-CG-OD2	6.06	123.76	118.30
2	M	10	ASP	CB-CG-OD2	6.03	123.72	118.30
2	K	149	ASP	CB-CG-OD2	6.01	123.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	114	ASP	CB-CG-OD1	5.97	123.67	118.30
3	R	189	ASP	CB-CG-OD2	5.92	123.62	118.30
1	D	84	ASP	CB-CG-OD1	5.90	123.61	118.30
2	N	182	ASP	CB-CG-OD2	5.88	123.59	118.30
1	F	170	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	51	ASP	CB-CG-OD2	5.78	123.50	118.30
3	O	189	ASP	CB-CG-OD2	5.77	123.50	118.30
3	T	223	ARG	NE-CZ-NH2	-5.77	117.42	120.30
2	M	195	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	18	ASP	CB-CG-OD2	5.76	123.48	118.30
2	L	27	MET	CG-SD-CE	5.74	109.38	100.20
3	R	227	ASP	CB-CG-OD2	5.66	123.39	118.30
2	N	166	ASP	CB-CG-OD2	5.63	123.37	118.30
2	L	195	ARG	NE-CZ-NH2	-5.63	117.49	120.30
3	R	157	ASP	CB-CG-OD2	5.62	123.36	118.30
2	H	18	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	I	51	ASP	CB-CG-OD2	5.60	123.34	118.30
1	G	18	ASP	CB-CG-OD2	5.59	123.33	118.30
2	L	10	ASP	CB-CG-OD2	5.57	123.32	118.30
1	F	225	ASP	CB-CG-OD2	5.57	123.31	118.30
1	G	90	ASP	CB-CG-OD2	5.57	123.31	118.30
3	S	103	ASP	CB-CG-OD2	5.52	123.27	118.30
2	N	105	ASP	CB-CG-OD2	5.51	123.26	118.30
2	J	51	ASP	CB-CG-OD2	5.41	123.17	118.30
2	L	114	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	51	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	51	ASP	CB-CG-OD2	5.38	123.14	118.30
2	J	10	ASP	CB-CG-OD2	5.38	123.14	118.30
2	I	182	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	51	ASP	CB-CG-OD2	5.34	123.11	118.30
1	E	152	ASP	CB-CG-OD2	5.31	123.08	118.30
1	E	170	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	72	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	225	ASP	CB-CG-OD2	5.22	123.00	118.30
2	K	70	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	I	10	ASP	CB-CG-OD2	5.18	122.96	118.30
2	H	190	ASP	CB-CG-OD2	5.18	122.96	118.30
3	S	77	LEU	CA-CB-CG	-5.18	103.40	115.30
2	H	114	ASP	CB-CG-OD2	5.17	122.96	118.30
2	K	122	ASP	CB-CG-OD2	5.17	122.95	118.30
2	L	203	LEU	CB-CG-CD2	5.16	119.76	111.00
2	K	190	ASP	CB-CG-OD2	5.15	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	14	ASP	CB-CG-OD2	5.15	122.93	118.30
2	H	166	ASP	CB-CG-OD2	5.14	122.93	118.30
2	N	114	ASP	CB-CG-OD1	5.13	122.92	118.30
3	Q	189	ASP	CB-CG-OD2	5.13	122.92	118.30
3	Q	227	ASP	CB-CG-OD2	5.10	122.89	118.30
3	Q	14	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	88	LEU	CB-CG-CD1	5.07	119.61	111.00
2	K	166	ASP	CB-CG-OD2	5.06	122.86	118.30
1	C	150	ASP	CB-CG-OD1	5.06	122.85	118.30
2	L	182	ASP	CB-CG-OD2	5.05	122.85	118.30
2	M	182	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	142	ASP	CB-CG-OD2	5.03	122.83	118.30
2	J	149	ASP	CB-CG-OD2	5.02	122.82	118.30
2	J	190	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	62	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1728	0	1764	54	0
1	B	1728	0	1764	44	0
1	C	1728	0	1764	41	0
1	D	1728	0	1764	45	0
1	E	1728	0	1764	54	0
1	F	1728	0	1764	38	0
1	G	1728	0	1764	32	0
2	H	1577	0	1625	27	0
2	I	1577	0	1625	29	0
2	J	1577	0	1625	24	0
2	K	1569	0	1617	30	0
2	L	1569	0	1617	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1577	0	1625	33	0
2	N	1577	0	1625	28	0
3	O	1679	0	1700	32	0
3	P	1679	0	1700	28	0
3	Q	1679	0	1700	32	0
3	R	1679	0	1700	34	0
3	S	1679	0	1700	32	0
3	T	1679	0	1700	38	0
3	U	1679	0	1700	36	0
4	A	5	0	0	2	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	10	0	0	0	0
4	I	15	0	0	1	0
4	J	10	0	0	1	0
4	K	10	0	0	0	0
4	L	10	0	0	1	0
4	M	20	0	0	1	0
4	N	15	0	0	1	0
5	H	6	0	8	0	0
5	I	6	0	8	0	0
5	J	6	0	8	0	0
5	K	6	0	8	0	0
5	L	6	0	8	2	0
5	M	6	0	8	0	0
5	N	6	0	8	0	0
6	A	67	0	0	7	0
6	B	58	0	0	2	0
6	C	69	0	0	2	0
6	D	49	0	0	3	0
6	E	67	0	0	10	0
6	F	61	0	0	5	0
6	G	51	0	0	3	0
6	H	93	0	0	3	0
6	I	100	0	0	9	0
6	J	94	0	0	14	0
6	K	85	0	0	12	0
6	L	93	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	100	0	0	6	0
6	N	107	0	0	8	0
6	O	52	0	0	3	0
6	P	47	0	0	2	0
6	Q	47	0	0	1	0
6	R	69	0	0	4	0
6	S	90	0	0	1	0
6	T	97	0	0	1	0
6	U	75	0	0	5	0
All	All	36610	0	35663	652	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (652) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:184:ARG:HH11	3:U:184:ARG:HG2	0.95	1.11
1:E:143:GLN:HG3	6:E:3051:HOH:O	1.49	1.10
1:D:28:ARG:HH22	3:U:229:MET:HG2	1.02	1.08
2:L:27:MET:HG2	6:M:3108:HOH:O	1.53	1.08
1:G:28:ARG:HH22	3:Q:229:MET:HG2	1.20	1.05
1:E:28:ARG:HH22	3:O:229:MET:HG2	1.16	1.04
3:R:184:ARG:HB3	3:R:184:ARG:HH11	1.18	1.03
3:O:89:ARG:HB3	3:O:89:ARG:HH11	1.20	1.03
1:E:106:LEU:HD21	6:E:3071:HOH:O	1.60	1.01
2:I:22:MET:HE1	6:J:3103:HOH:O	1.60	1.00
3:S:144:ALA:HB3	6:S:320:HOH:O	1.59	1.00
1:E:208:LYS:CD	1:E:208:LYS:H	1.73	0.99
1:C:13:THR:O	1:D:130:ARG:HB3	1.63	0.98
3:U:184:ARG:HG2	3:U:184:ARG:NH1	1.72	0.98
1:A:106:LEU:HD21	6:A:3049:HOH:O	1.63	0.97
3:O:89:ARG:HB3	3:O:89:ARG:NH1	1.81	0.96
2:I:9:LYS:HE3	6:I:3095:HOH:O	1.66	0.96
1:B:28:ARG:HH22	3:S:229:MET:HG3	1.30	0.95
1:A:12:ILE:HG13	1:A:13:THR:HG23	1.45	0.95
1:B:62:ASN:H	1:B:62:ASN:HD22	1.00	0.94
1:E:208:LYS:HD2	1:E:208:LYS:H	1.32	0.93
2:J:203:LEU:HD21	6:J:3101:HOH:O	1.68	0.91
1:B:90:ASP:HB3	6:H:3078:HOH:O	1.69	0.91
1:D:28:ARG:NH2	3:U:229:MET:HG2	1.86	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ARG:HH22	3:U:229:MET:CG	1.85	0.90
2:J:22:MET:HB2	2:J:27:MET:SD	2.11	0.90
2:J:203:LEU:CD2	6:J:3101:HOH:O	2.20	0.89
3:R:184:ARG:CB	3:R:184:ARG:HH11	1.86	0.88
1:G:12:ILE:HA	1:G:23:GLN:HG3	1.56	0.87
2:M:58[A]:TYR:HD2	2:M:59:MET:HE2	1.38	0.87
3:T:89:ARG:HD2	3:U:203:THR:HG21	1.56	0.86
1:B:12:ILE:HG13	1:B:13:THR:HG23	1.56	0.86
1:E:28:ARG:HH22	3:O:229:MET:CG	1.89	0.85
1:E:201:LEU:O	1:E:202:GLU:HB2	1.76	0.85
2:L:22:MET:HB2	2:L:27:MET:SD	2.17	0.84
1:C:61:GLN:CD	1:C:61:GLN:H	1.80	0.84
2:M:172:MET:HA	2:M:172:MET:HE3	1.60	0.83
2:H:9:LYS:HG3	6:H:3025:HOH:O	1.76	0.83
1:B:62:ASN:N	1:B:62:ASN:HD22	1.71	0.83
3:R:184:ARG:HB3	3:R:184:ARG:NH1	1.93	0.82
1:F:13:THR:O	1:G:130:ARG:HB3	1.78	0.82
1:B:62:ASN:ND2	1:B:62:ASN:H	1.77	0.82
2:M:58[A]:TYR:CD2	2:M:59:MET:HE2	2.15	0.82
2:I:9:LYS:HG3	6:I:3107:HOH:O	1.78	0.82
2:I:27:MET:CE	6:J:3098:HOH:O	2.28	0.82
1:G:90:ASP:HB3	6:M:3091:HOH:O	1.80	0.81
3:Q:119:GLU:HG3	3:Q:123:LYS:HE3	1.63	0.80
1:B:28:ARG:NH2	3:S:229:MET:HG3	1.97	0.80
1:B:175:PHE:CZ	1:B:195:LYS:HG2	2.15	0.79
1:D:65:GLU:HA	6:D:3022:HOH:O	1.80	0.79
1:A:12:ILE:HG23	6:A:3029:HOH:O	1.82	0.79
1:A:130:ARG:HB3	1:G:13:THR:O	1.81	0.79
1:F:28:ARG:HH22	3:P:229:MET:CG	1.95	0.78
1:A:13:THR:O	1:B:130:ARG:HB3	1.82	0.78
3:T:116:ILE:HG12	3:T:204:MET:CE	2.14	0.78
6:F:3054:HOH:O	1:G:64:ILE:HD12	1.83	0.78
1:D:13:THR:O	1:E:130:ARG:HB3	1.83	0.77
1:F:12:ILE:HG13	1:F:13:THR:HG23	1.66	0.77
1:B:222:ARG:NH1	1:B:228:GLU:OE1	2.18	0.77
2:M:186:GLN:OE1	6:M:3124:HOH:O	2.02	0.77
2:K:186:GLN:HG3	6:K:3072:HOH:O	1.84	0.76
2:L:191:GLN:HE21	2:L:195:ARG:HE	1.33	0.76
1:D:12:ILE:HG13	1:D:13:THR:HG23	1.67	0.75
2:I:27:MET:HE1	6:J:3098:HOH:O	1.87	0.74
1:G:64:ILE:HG12	6:G:3019:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:ILE:HG13	1:G:13:THR:HG23	1.67	0.74
1:D:12:ILE:HA	1:D:23:GLN:HG3	1.69	0.74
1:F:12:ILE:HA	1:F:23:GLN:HG3	1.68	0.74
1:D:90:ASP:HB3	6:J:3069:HOH:O	1.87	0.73
3:T:116:ILE:HG12	3:T:204:MET:HE3	1.70	0.72
1:C:107:VAL:HG13	1:C:143:GLN:HG3	1.70	0.72
2:J:27:MET:HG2	6:K:3044:HOH:O	1.90	0.72
4:J:3017:SO4:O1	6:J:3110:HOH:O	2.08	0.71
3:O:132:GLY:HA3	6:O:255:HOH:O	1.90	0.71
1:A:52:LYS:NZ	1:A:66:LYS:HD2	2.06	0.70
3:R:144:ALA:HB3	6:R:286:HOH:O	1.91	0.70
1:E:28:ARG:NH2	6:E:3056:HOH:O	2.23	0.70
2:M:58[A]:TYR:HD2	2:M:59:MET:CE	2.03	0.70
2:N:24:ASN:H	2:N:24:ASN:HD22	1.37	0.70
1:E:222:ARG:NH1	1:E:228:GLU:OE2	2.16	0.70
3:Q:89:ARG:NH1	3:Q:118:ASP:OD1	2.25	0.70
1:A:81:LEU:HD23	3:Q:230:VAL:HG22	1.73	0.70
3:R:56:GLY:H	3:R:59:GLN:HE21	1.40	0.69
2:J:157:ARG:HD2	6:J:3028:HOH:O	1.92	0.69
1:C:12:ILE:HG13	1:C:13:THR:HG23	1.73	0.69
2:I:163:LYS:NZ	2:I:203:LEU:HB3	2.08	0.69
2:N:67:ARG:HD2	6:N:3075:HOH:O	1.91	0.69
3:Q:133:SER:HB3	3:R:133:SER:HB2	1.72	0.69
1:A:187:LYS:HE3	1:A:231:LYS:NZ	2.07	0.69
2:J:197:ARG:HG2	6:J:3107:HOH:O	1.92	0.69
6:G:3010:HOH:O	3:Q:229:MET:SD	2.51	0.69
3:U:184:ARG:HH11	3:U:184:ARG:CG	1.89	0.68
1:F:28:ARG:HH22	3:P:229:MET:HG2	1.57	0.68
2:H:18:ARG:CZ	2:H:174:ASP:OD1	2.41	0.68
2:N:202:ILE:HG13	2:N:203:LEU:H	1.59	0.68
3:R:221:GLN:HG3	6:R:289:HOH:O	1.93	0.68
1:F:12:ILE:N	6:F:3046:HOH:O	2.26	0.68
2:M:58[A]:TYR:CD2	2:M:59:MET:CE	2.76	0.68
3:O:97:PRO:HG3	3:O:222:PRO:HG2	1.76	0.68
1:E:61:GLN:NE2	1:E:62:ASN:H	1.92	0.68
4:I:3016:SO4:O4	6:I:3118:HOH:O	2.09	0.67
2:N:172:MET:CE	2:N:173:ILE:H	2.07	0.67
2:M:157:ARG:HD2	6:M:3046:HOH:O	1.93	0.67
2:H:163:LYS:NZ	2:H:203:LEU:HB3	2.08	0.67
2:I:9:LYS:HG2	6:I:3040:HOH:O	1.93	0.66
1:C:28:ARG:HH12	3:T:229:MET:HG3	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:172:MET:HE3	2:N:173:ILE:H	1.60	0.66
2:H:22:MET:HE1	6:I:3066:HOH:O	1.95	0.66
1:G:28:ARG:NH2	3:Q:229:MET:HG2	2.04	0.66
2:I:187:LEU:HB2	2:I:192:ILE:HD11	1.78	0.66
1:E:28:ARG:NH2	3:O:229:MET:HG2	2.01	0.66
2:H:32:LYS:HE2	6:H:3087:HOH:O	1.95	0.65
1:E:51:ASP:OD1	6:E:3066:HOH:O	2.14	0.65
1:C:33:LYS:HB2	3:S:230:VAL:HG11	1.78	0.65
2:K:144:GLU:HG2	6:K:3068:HOH:O	1.97	0.65
1:B:12:ILE:HA	1:B:23:GLN:HG3	1.79	0.65
3:T:146:ARG:HD3	6:U:240:HOH:O	1.97	0.65
3:P:64:PRO:HB2	3:P:67:LEU:HG	1.78	0.64
1:A:187:LYS:HE3	1:A:231:LYS:HZ1	1.60	0.64
3:Q:129:GLU:HG2	3:R:138:THR:O	1.97	0.64
1:D:230:LYS:HA	1:D:233:LEU:HD12	1.79	0.64
3:T:11:ASN:OD1	6:T:322:HOH:O	2.15	0.64
1:B:28:ARG:NH2	3:S:229:MET:CG	2.61	0.64
3:P:149:LEU:O	3:P:153:SER:HB3	1.97	0.64
1:C:12:ILE:HA	1:C:23:GLN:HG3	1.80	0.64
3:T:64:PRO:O	3:T:68:LEU:HG	1.98	0.64
2:N:201:LEU:O	6:N:3123:HOH:O	2.15	0.64
1:A:90:ASP:HB3	6:N:3111:HOH:O	1.98	0.63
1:E:71:ASP:HA	2:K:68:LEU:HD21	1.81	0.63
2:N:172:MET:HA	2:N:172:MET:HE3	1.80	0.63
1:C:209:ALA:CB	1:C:233:LEU:HD11	2.29	0.63
2:L:191:GLN:HB2	6:L:3104:HOH:O	1.98	0.63
1:C:106:LEU:HD21	6:C:3071:HOH:O	1.99	0.63
1:C:62:ASN:H	1:C:62:ASN:ND2	1.96	0.63
2:K:18:ARG:HG3	2:K:172:MET:O	1.99	0.63
3:O:192:LEU:HD21	3:U:142:MET:HE1	1.80	0.62
2:L:18:ARG:NH1	2:L:30:ASN:OD1	2.30	0.62
2:L:105:ASP:O	2:L:180:ARG:NH1	2.31	0.62
2:J:157:ARG:CD	6:J:3028:HOH:O	2.47	0.62
1:F:62:ASN:HD22	1:F:62:ASN:H	1.47	0.62
3:P:63:SER:HG	3:Q:178:SER:HG	1.44	0.62
1:E:41:LYS:NZ	1:F:60:GLU:OE2	2.32	0.61
1:B:62:ASN:N	1:B:62:ASN:ND2	2.43	0.61
1:F:28:ARG:HH22	3:P:229:MET:HG3	1.65	0.61
3:S:189:ASP:O	3:S:193:LYS:HG3	1.99	0.61
1:A:203:GLU:CD	1:A:203:GLU:H	2.03	0.61
1:A:65:GLU:HA	4:A:3007:SO4:O1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:ILE:HD12	1:F:211:GLU:HG2	1.82	0.61
3:P:28:TRP:HA	3:P:32:THR:HB	1.83	0.61
1:D:187:LYS:HE3	1:D:232:PHE:CE2	2.34	0.61
1:D:178:ARG:HG2	1:D:179:GLU:HG2	1.82	0.61
2:H:91:LYS:HE2	2:N:51:ASP:OD1	2.00	0.61
2:H:24:ASN:HD22	2:H:24:ASN:H	1.48	0.61
1:D:12:ILE:HG13	1:D:13:THR:CG2	2.30	0.60
3:R:89:ARG:HD3	3:R:121:GLU:OE2	2.01	0.60
2:N:202:ILE:CG1	2:N:203:LEU:H	2.13	0.60
1:E:208:LYS:N	1:E:208:LYS:HD2	2.12	0.60
1:C:209:ALA:HA	1:C:233:LEU:HD11	1.84	0.60
2:L:43:MET:HE2	2:L:56:VAL:HG22	1.83	0.60
2:M:40:TYR:CD1	2:M:183:GLY:HA2	2.37	0.60
2:H:18:ARG:NH2	2:H:174:ASP:OD1	2.35	0.60
1:G:141:ILE:HD12	1:G:215:ILE:HG12	1.84	0.59
2:I:98:GLN:HB3	6:I:3119:HOH:O	2.01	0.59
2:J:203:LEU:HD23	6:J:3101:HOH:O	1.97	0.59
1:C:55:ARG:HA	1:C:55:ARG:CZ	2.32	0.59
3:R:184:ARG:HH11	3:R:184:ARG:CG	2.15	0.59
1:G:201:LEU:HD21	6:G:3040:HOH:O	2.02	0.59
1:B:202:GLU:O	1:B:205:GLU:HB3	2.02	0.59
3:T:116:ILE:HG12	3:T:204:MET:HE1	1.84	0.59
2:L:43:MET:CE	2:L:56:VAL:HG22	2.32	0.59
1:G:28:ARG:HH22	3:Q:229:MET:CG	2.07	0.59
1:A:52:LYS:HZ2	1:A:66:LYS:HD2	1.65	0.59
3:P:63:SER:OG	3:Q:178:SER:OG	2.14	0.59
3:T:86:GLU:OE2	3:T:121:GLU:OE1	2.20	0.59
1:A:66:LYS:HE3	1:A:66:LYS:HA	1.83	0.59
1:F:62:ASN:N	1:F:62:ASN:HD22	2.01	0.59
1:A:12:ILE:CG1	1:A:13:THR:HG23	2.26	0.58
1:C:28:ARG:NH2	1:C:152:ASP:OD2	2.31	0.58
1:A:12:ILE:HD12	1:A:12:ILE:O	2.03	0.58
1:G:12:ILE:HA	1:G:23:GLN:CG	2.31	0.58
1:D:107:VAL:O	1:D:142:ASP:HB2	2.03	0.58
2:K:2:THR:OG1	2:K:130:GLY:HA3	2.04	0.58
1:A:28:ARG:NH2	1:A:152:ASP:OD2	2.34	0.58
6:A:3033:HOH:O	1:B:82:VAL:HG11	2.03	0.58
1:F:51:ASP:HB2	1:F:197:LEU:HD11	1.85	0.58
1:F:106:LEU:HD21	6:F:3060:HOH:O	2.02	0.58
3:O:192:LEU:HD21	3:U:142:MET:CE	2.33	0.58
3:R:140:ILE:CD1	3:R:144:ALA:HB1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:24:ASN:H	2:N:24:ASN:ND2	2.00	0.58
3:S:50:ILE:HD11	3:S:67:LEU:HD21	1.85	0.58
2:L:18:ARG:NE	2:L:174:ASP:OD1	2.33	0.58
3:U:50:ILE:HD11	3:U:67:LEU:HD21	1.85	0.58
1:D:12:ILE:HG12	1:D:129:VAL:O	2.03	0.58
1:E:13:THR:HG22	6:E:3011:HOH:O	2.04	0.58
3:S:143:TYR:O	3:S:147:GLU:HG3	2.03	0.58
1:F:201:LEU:O	1:F:202:GLU:O	2.22	0.57
2:N:91:LYS:HE2	6:N:3110:HOH:O	2.03	0.57
2:J:18:ARG:HH21	2:J:30:ASN:HD21	1.52	0.57
1:E:208:LYS:HD3	1:E:208:LYS:H	1.66	0.57
2:J:18:ARG:HD2	2:J:31:GLY:O	2.05	0.57
2:H:163:LYS:HZ1	2:H:203:LEU:HB3	1.66	0.57
2:K:37:ILE:HG21	2:K:43:MET:HE2	1.86	0.57
2:K:24:ASN:H	2:K:24:ASN:HD22	1.53	0.57
1:A:186:GLU:O	1:A:190:VAL:HG23	2.05	0.56
2:H:194:SER:O	2:H:198:LYS:HG2	2.04	0.56
1:B:28:ARG:HH22	3:S:229:MET:CG	2.09	0.56
3:Q:50:ILE:HD11	3:Q:67:LEU:HD11	1.87	0.56
1:A:107:VAL:HG13	1:A:143:GLN:HG3	1.86	0.56
3:O:73:ARG:HD2	6:O:247:HOH:O	2.06	0.56
1:C:61:GLN:C	1:C:63:SER:H	2.09	0.56
3:T:89:ARG:NH2	3:T:118:ASP:OD1	2.39	0.56
1:E:227:GLU:O	1:E:231:LYS:HD3	2.06	0.56
1:E:156:THR:HG23	1:F:82:VAL:HG21	1.87	0.56
2:H:147:THR:OG1	2:H:150:GLU:HG2	2.05	0.56
2:H:172:MET:HE3	2:H:192:ILE:HG21	1.87	0.55
1:B:175:PHE:HZ	1:B:195:LYS:HG2	1.69	0.55
1:A:28:ARG:HH22	3:R:229:MET:HG3	1.71	0.55
2:I:2:THR:OG1	2:I:130:GLY:HA3	2.06	0.55
2:M:18:ARG:HG3	2:M:172:MET:O	2.06	0.55
2:J:17:GLU:C	2:J:18:ARG:HG2	2.26	0.55
1:E:61:GLN:H	1:E:61:GLN:CD	2.09	0.55
3:P:65:GLU:HA	3:P:68:LEU:HD12	1.88	0.55
2:J:24:ASN:HD22	2:J:24:ASN:H	1.53	0.55
1:A:94:ILE:O	1:A:98:GLN:HG3	2.05	0.55
1:D:180:TYR:HA	1:D:192:LEU:HD21	1.87	0.55
1:D:13:THR:HG21	1:D:126:TYR:C	2.27	0.55
1:B:222:ARG:HH12	1:B:228:GLU:CD	2.10	0.55
2:J:157:ARG:NE	6:J:3097:HOH:O	2.38	0.55
2:M:163:LYS:HZ1	2:M:203:LEU:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ILE:HD12	1:E:211:GLU:HB3	1.86	0.55
3:O:89:ARG:CB	3:O:89:ARG:NH1	2.63	0.55
2:H:24:ASN:ND2	2:H:24:ASN:H	2.05	0.55
1:F:142:ASP:OD2	1:F:147:ARG:NH1	2.37	0.55
1:E:100:LYS:NZ	6:E:3033:HOH:O	2.38	0.55
3:P:140:ILE:HG23	3:P:193:LYS:HD3	1.88	0.55
3:T:89:ARG:CD	3:U:203:THR:HG21	2.33	0.55
1:D:107:VAL:HG13	1:D:143:GLN:CG	2.37	0.55
3:S:101:GLU:HG3	3:T:105:LEU:CD2	2.37	0.55
2:M:18:ARG:NH1	2:M:174:ASP:OD2	2.40	0.54
1:E:33:LYS:HB2	3:U:230:VAL:HG11	1.89	0.54
2:M:1:THR:HB	4:M:3010:SO4:O3	2.07	0.54
1:E:209:ALA:HA	1:E:233:LEU:HD11	1.88	0.54
1:F:71:ASP:HA	2:L:68:LEU:HD21	1.89	0.54
1:C:61:GLN:O	1:C:63:SER:N	2.38	0.54
1:A:63:SER:HB2	1:G:159:GLU:OE1	2.07	0.54
3:P:24:VAL:HG13	3:P:84:GLN:HB3	1.90	0.54
3:R:28:TRP:HA	3:R:32:THR:HB	1.89	0.54
3:U:89:ARG:HD3	3:U:117:ILE:HG22	1.89	0.54
1:A:12:ILE:N	6:A:3074:HOH:O	2.40	0.54
1:A:175:PHE:CZ	1:A:179:GLU:HG3	2.43	0.54
6:Q:274:HOH:O	3:R:18:GLU:HG2	2.07	0.54
2:I:163:LYS:HZ1	2:I:203:LEU:HB3	1.73	0.54
3:O:133:SER:N	3:P:133:SER:O	2.39	0.54
3:O:11:ASN:O	3:O:15:SER:HB3	2.08	0.54
1:F:12:ILE:HG13	1:F:13:THR:CG2	2.38	0.53
3:O:65:GLU:HA	3:O:68:LEU:HD12	1.89	0.53
3:U:75:GLN:HG3	3:U:142:MET:O	2.08	0.53
3:O:73:ARG:CD	6:O:247:HOH:O	2.55	0.53
3:T:89:ARG:NH1	3:T:118:ASP:OD1	2.38	0.53
1:D:126:TYR:HH	1:E:123:TYR:HH	1.56	0.53
3:O:51:ARG:NH2	3:U:76:ASP:OD1	2.41	0.53
1:C:222:ARG:HB2	1:C:222:ARG:HH11	1.74	0.53
3:Q:75:GLN:HG3	3:Q:142:MET:O	2.08	0.53
3:Q:181:LEU:O	3:Q:184:ARG:HB3	2.09	0.53
1:C:208:LYS:O	1:C:209:ALA:CB	2.57	0.52
3:S:101:GLU:HG3	3:T:105:LEU:HD22	1.91	0.52
1:C:13:THR:O	1:D:130:ARG:CB	2.47	0.52
1:F:55:ARG:O	1:F:56:SER:CB	2.56	0.52
2:K:18:ARG:HD3	2:K:174:ASP:OD2	2.10	0.52
3:Q:50:ILE:HD13	3:Q:187:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:THR:HG23	1:F:82:VAL:CG2	2.40	0.52
1:A:61:GLN:O	1:A:62:ASN:CB	2.57	0.52
2:M:82:LEU:HG	2:M:86:MET:CE	2.39	0.52
1:F:12:ILE:HA	1:F:23:GLN:CG	2.39	0.52
3:R:82:TYR:CD2	3:S:196:LEU:HD22	2.45	0.52
1:D:12:ILE:CD1	1:D:13:THR:HG22	2.40	0.52
2:J:52:ALA:O	2:J:56:VAL:HG23	2.09	0.52
2:N:32:LYS:HE3	6:N:3047:HOH:O	2.09	0.52
3:T:65:GLU:HA	3:T:68:LEU:HD12	1.92	0.52
3:P:97:PRO:HG3	3:P:222:PRO:HG2	1.92	0.52
6:F:3054:HOH:O	1:G:64:ILE:HG23	2.10	0.51
3:Q:101:GLU:HG3	3:R:105:LEU:CD2	2.41	0.51
1:C:13:THR:HG21	1:C:126:TYR:C	2.31	0.51
1:C:61:GLN:CD	1:C:61:GLN:N	2.58	0.51
3:P:28:TRP:HB3	3:P:209:ILE:HD11	1.92	0.51
2:J:18:ARG:NH2	2:J:30:ASN:HD21	2.08	0.51
3:R:56:GLY:H	3:R:59:GLN:NE2	2.07	0.51
1:B:173:VAL:O	1:B:177:GLU:HG3	2.10	0.51
2:K:80:ALA:O	2:K:84:SER:HB3	2.10	0.51
1:D:107:VAL:HG13	1:D:143:GLN:HG3	1.93	0.51
3:S:101:GLU:CG	3:T:105:LEU:HD22	2.41	0.51
1:G:71:ASP:HB2	2:M:64:GLU:OE2	2.11	0.51
1:A:65:GLU:HB3	4:A:3007:SO4:O4	2.11	0.51
2:L:24:ASN:H	2:L:24:ASN:HD22	1.59	0.51
2:M:18:ARG:HD2	2:M:31:GLY:O	2.11	0.51
3:O:36:ILE:HG23	3:O:198:THR:HB	1.93	0.51
1:E:201:LEU:O	1:E:202:GLU:CB	2.53	0.51
3:R:144:ALA:O	3:R:147:GLU:HB2	2.11	0.51
1:F:13:THR:HG21	1:F:126:TYR:C	2.32	0.50
2:J:45:ILE:HB	2:J:52:ALA:HB1	1.93	0.50
3:S:129:GLU:HG3	3:T:138:THR:O	2.11	0.50
1:A:13:THR:O	1:B:130:ARG:CB	2.57	0.50
1:E:77:VAL:HG12	1:E:137:ILE:HB	1.92	0.50
1:D:152:ASP:HB2	1:D:153:PRO:HD2	1.92	0.50
1:A:76:ALA:HA	1:A:137:ILE:O	2.11	0.50
1:A:12:ILE:HB	6:A:3031:HOH:O	2.10	0.50
2:I:80:ALA:O	2:I:84:SER:HB3	2.10	0.50
1:E:64:ILE:HA	6:E:3065:HOH:O	2.10	0.50
2:M:24:ASN:H	2:M:24:ASN:HD22	1.59	0.50
1:A:33:LYS:HB2	3:Q:230:VAL:HG11	1.94	0.50
3:U:184:ARG:NH1	3:U:184:ARG:CG	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:9:ILE:HD11	3:S:213:LEU:HB2	1.93	0.50
2:M:17:GLU:C	2:M:18:ARG:HG2	2.32	0.50
1:D:12:ILE:O	1:D:12:ILE:HD12	2.12	0.50
2:K:45:ILE:HB	2:K:52:ALA:HB1	1.93	0.50
1:A:13:THR:O	1:B:130:ARG:HD3	2.12	0.50
1:D:71:ASP:HB2	2:J:64:GLU:OE2	2.12	0.50
3:S:28:TRP:HA	3:S:32:THR:HB	1.93	0.50
1:G:55:ARG:O	1:G:56:SER:CB	2.60	0.50
2:L:62:GLU:HG2	2:L:82:LEU:HD21	1.93	0.50
2:I:87:LEU:HD23	2:I:95:TYR:CD1	2.47	0.49
2:L:45:ILE:HB	2:L:52:ALA:HB1	1.93	0.49
1:C:28:ARG:HH22	3:T:229:MET:CG	2.25	0.49
3:Q:64:PRO:HB2	3:Q:67:LEU:HG	1.94	0.49
2:I:30:ASN:CG	6:I:3038:HOH:O	2.50	0.49
3:U:225:GLY:HA3	6:U:290:HOH:O	2.11	0.49
3:U:36:ILE:HG23	3:U:198:THR:HB	1.94	0.49
1:A:212:ILE:HD12	1:A:229:VAL:HG22	1.93	0.49
1:A:50:SER:OG	1:A:66:LYS:HG2	2.13	0.49
1:A:21:LEU:HD12	3:R:229:MET:CE	2.43	0.49
2:M:2:THR:OG1	2:M:130:GLY:HA3	2.13	0.49
2:K:18:ARG:HD2	6:K:3054:HOH:O	2.12	0.49
1:D:71:ASP:HA	2:J:68:LEU:HD21	1.94	0.49
3:O:140:ILE:CD1	3:O:144:ALA:HB1	2.43	0.49
1:F:55:ARG:O	1:F:56:SER:HB2	2.12	0.49
2:I:24:ASN:H	2:I:24:ASN:HD22	1.61	0.49
1:F:12:ILE:HG23	6:F:3039:HOH:O	2.13	0.49
1:C:209:ALA:HB2	1:C:233:LEU:HD11	1.94	0.49
1:C:55:ARG:HA	1:C:55:ARG:NH1	2.28	0.49
3:Q:90:THR:O	3:Q:94:ILE:HG12	2.12	0.49
1:B:12:ILE:CG1	1:B:13:THR:HG23	2.38	0.48
2:N:163:LYS:NZ	2:N:203:LEU:CB	2.76	0.48
2:I:45:ILE:HB	2:I:52:ALA:HB1	1.94	0.48
2:H:124:TYR:CD1	2:H:138:LEU:HD13	2.48	0.48
2:K:51:ASP:OD1	2:L:91:LYS:HE2	2.13	0.48
1:E:210:PRO:HD2	1:E:229:VAL:CG1	2.43	0.48
2:N:18:ARG:HG3	2:N:172:MET:O	2.14	0.48
2:M:32:LYS:HE3	2:M:35:PHE:CE1	2.48	0.48
2:J:202:ILE:HD13	2:J:202:ILE:H	1.79	0.48
1:E:65:GLU:O	1:E:68:GLN:NE2	2.46	0.48
1:F:176:LEU:O	1:F:180:TYR:CB	2.62	0.48
1:F:176:LEU:O	1:F:180:TYR:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LYS:HA	1:B:201:LEU:HD22	1.95	0.48
1:F:12:ILE:O	1:F:12:ILE:HD12	2.14	0.48
1:C:209:ALA:CA	1:C:233:LEU:HD11	2.44	0.48
2:K:163:LYS:HB3	2:K:203:LEU:HD22	1.96	0.48
1:E:83:ALA:HB3	6:E:3026:HOH:O	2.14	0.48
1:A:63:SER:CB	1:G:159:GLU:OE1	2.62	0.48
1:G:180:TYR:HA	1:G:192:LEU:HD21	1.95	0.48
3:U:4:LYS:HA	6:U:289:HOH:O	2.14	0.48
2:M:74:MET:HG2	2:M:78:ALA:HB3	1.96	0.48
3:T:105:LEU:O	3:T:109:VAL:HG23	2.14	0.47
2:K:9:LYS:HG3	6:K:3029:HOH:O	2.13	0.47
2:I:163:LYS:HZ3	2:I:203:LEU:HB3	1.78	0.47
2:M:36:GLN:O	2:M:60:LYS:HE2	2.15	0.47
3:S:140:ILE:HB	3:S:193:LYS:HB3	1.97	0.47
1:B:110:GLU:HG3	1:B:149:PHE:CE2	2.50	0.47
2:L:53:GLN:HB3	5:L:2001:GOL:H12	1.97	0.47
3:O:24:VAL:HG13	3:O:84:GLN:HB3	1.96	0.47
3:Q:140:ILE:HG13	3:Q:144:ALA:HB2	1.95	0.47
3:R:140:ILE:HD11	3:R:144:ALA:HB1	1.96	0.47
1:A:18:ASP:HB2	3:R:102:GLU:OE1	2.14	0.47
3:S:124:THR:HG23	3:S:200:HIS:HD2	1.80	0.47
2:M:27:MET:HG2	6:N:3066:HOH:O	2.15	0.47
3:T:160:LEU:O	3:T:161:GLY:C	2.51	0.47
1:C:24:VAL:HG11	1:C:154:ALA:HB2	1.95	0.47
3:U:132:GLY:HA3	6:U:264:HOH:O	2.14	0.47
1:F:209:ALA:HA	1:F:233:LEU:HD11	1.96	0.47
2:I:91:LYS:HE3	2:I:92:TYR:CE1	2.49	0.47
2:I:93:MET:HE1	6:I:3116:HOH:O	2.14	0.47
3:P:71:LEU:HB2	3:P:145:LEU:HD13	1.97	0.47
1:B:65:GLU:O	1:B:68:GLN:NE2	2.48	0.47
1:G:149:PHE:HA	1:G:158:ASN:O	2.14	0.47
1:E:66:LYS:HB2	6:E:3062:HOH:O	2.15	0.47
3:O:50:ILE:HD11	3:O:67:LEU:HD21	1.96	0.47
2:L:22:MET:HE1	6:M:3121:HOH:O	2.15	0.47
2:I:87:LEU:HD23	2:I:95:TYR:HD1	1.80	0.47
6:E:3038:HOH:O	1:F:12:ILE:HB	2.15	0.46
1:D:13:THR:HG21	1:D:126:TYR:O	2.16	0.46
1:B:180:TYR:HA	1:B:192:LEU:HD21	1.97	0.46
2:M:163:LYS:NZ	2:M:203:LEU:HB3	2.29	0.46
1:F:43:ALA:HA	1:F:183:ASN:OD1	2.15	0.46
3:P:89:ARG:NH1	3:P:118:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:152:VAL:O	2:I:156:ILE:HD12	2.14	0.46
2:K:157:ARG:HD2	6:K:3051:HOH:O	2.15	0.46
1:D:203:GLU:CD	1:D:203:GLU:N	2.69	0.46
2:H:82:LEU:O	2:H:86:MET:HG3	2.15	0.46
1:E:61:GLN:O	1:E:62:ASN:C	2.53	0.46
3:S:64:PRO:HB2	3:S:67:LEU:HG	1.98	0.46
2:N:59:MET:O	2:N:63:LEU:HG	2.16	0.46
1:B:186:GLU:O	1:B:190:VAL:HG23	2.14	0.46
1:A:201:LEU:HD11	1:A:207:LEU:HB2	1.96	0.46
1:A:67:ILE:HG12	1:A:77:VAL:CG1	2.45	0.46
1:E:81:LEU:HD23	3:U:230:VAL:CG2	2.46	0.46
3:O:133:SER:HB3	3:P:133:SER:HB2	1.97	0.46
2:K:203:LEU:HD11	6:K:3097:HOH:O	2.15	0.46
2:K:201:LEU:O	2:K:202:ILE:HG23	2.15	0.46
2:J:59:MET:CE	2:J:79:VAL:HG13	2.45	0.46
6:R:267:HOH:O	3:S:175:GLN:HG3	2.16	0.46
3:P:82:TYR:CD2	3:Q:196:LEU:HD22	2.50	0.46
2:K:24:ASN:ND2	2:K:24:ASN:H	2.14	0.46
3:Q:89:ARG:HD3	3:Q:121:GLU:OE2	2.15	0.46
2:N:18:ARG:HB3	2:N:30:ASN:HA	1.96	0.46
3:U:64:PRO:HB2	3:U:67:LEU:HG	1.98	0.46
3:S:61:GLU:C	3:T:177:PRO:HG3	2.36	0.46
1:D:42:PHE:HB2	1:D:184:LEU:O	2.16	0.46
1:A:225:ASP:OD2	1:A:227:GLU:HG2	2.15	0.46
1:C:162:ALA:HB1	1:C:176:LEU:HD13	1.97	0.46
1:B:66:LYS:HB2	1:B:211:GLU:OE2	2.15	0.46
1:B:51:ASP:HB2	1:B:197:LEU:HD11	1.98	0.46
1:C:61:GLN:C	1:C:63:SER:N	2.69	0.46
1:C:208:LYS:O	1:C:209:ALA:HB2	2.16	0.46
1:G:152:ASP:HB2	1:G:153:PRO:HD2	1.98	0.46
2:M:59:MET:HE1	2:M:86:MET:HE1	1.98	0.46
1:C:55:ARG:HB2	1:C:59:ILE:HG13	1.98	0.46
1:E:158:ASN:HB2	1:E:160:TYR:CE1	2.50	0.45
1:F:42:PHE:HB2	1:F:184:LEU:O	2.15	0.45
1:C:61:GLN:OE1	1:C:62:ASN:ND2	2.50	0.45
2:L:191:GLN:O	2:L:195:ARG:HG3	2.16	0.45
1:G:158:ASN:HB2	1:G:160:TYR:CE1	2.51	0.45
1:G:185:PRO:HG2	1:G:188:GLU:HB2	1.98	0.45
2:N:163:LYS:NZ	2:N:203:LEU:HB3	2.31	0.45
3:P:28:TRP:CB	3:P:209:ILE:HD11	2.46	0.45
2:H:23:GLU:HB3	2:H:24:ASN:H	1.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:172:MET:HE3	2:H:192:ILE:CG2	2.45	0.45
1:D:186:GLU:O	1:D:190:VAL:HG23	2.16	0.45
1:D:65:GLU:HG2	4:D:3003:SO4:O4	2.17	0.45
1:G:107:VAL:O	1:G:142:ASP:HB2	2.16	0.45
1:A:12:ILE:HA	1:A:23:GLN:HG3	1.97	0.45
1:B:13:THR:HG21	1:B:126:TYR:C	2.36	0.45
2:I:27:MET:HE3	6:J:3098:HOH:O	2.01	0.45
1:E:76:ALA:HA	1:E:137:ILE:O	2.16	0.45
1:D:203:GLU:CD	1:D:203:GLU:H	2.19	0.45
3:P:75:GLN:NE2	6:P:270:HOH:O	2.48	0.45
1:C:64:ILE:O	1:C:64:ILE:HG22	2.16	0.45
3:O:68:LEU:HD21	3:O:149:LEU:HD21	1.98	0.45
2:M:22:MET:HB2	2:M:27:MET:SD	2.57	0.45
1:E:24:VAL:HG11	1:E:154:ALA:HB2	1.99	0.45
3:P:50:ILE:HD11	3:P:67:LEU:HD21	1.98	0.45
3:S:63:SER:HA	3:S:64:PRO:HD3	1.80	0.45
1:B:180:TYR:O	1:B:181:LYS:HD2	2.16	0.45
2:I:172:MET:CE	2:I:192:ILE:HB	2.46	0.45
3:T:68:LEU:HD23	3:T:148:TYR:HE2	1.80	0.45
1:B:230:LYS:C	1:B:232:PHE:H	2.20	0.45
3:T:113:VAL:O	3:T:117:ILE:HG12	2.17	0.45
3:S:191:MET:O	3:S:195:GLU:HG3	2.16	0.45
2:L:163:LYS:HE2	2:L:203:LEU:HD13	1.99	0.45
2:M:98:GLN:HB3	6:M:3107:HOH:O	2.16	0.45
1:A:61:GLN:O	1:A:62:ASN:HB2	2.15	0.45
1:D:76:ALA:HA	1:D:137:ILE:O	2.17	0.45
2:L:70:ARG:NH1	4:L:3019:SO4:O1	2.49	0.45
3:O:80:ASN:O	3:O:84:GLN:HG3	2.17	0.45
1:B:71:ASP:HA	2:H:68:LEU:HD21	1.99	0.45
1:A:51:ASP:HB2	1:A:197:LEU:HD11	1.98	0.45
1:E:36:THR:HA	1:E:165:ILE:O	2.17	0.45
3:T:116:ILE:O	3:T:204:MET:CE	2.65	0.44
1:B:64:ILE:O	1:B:64:ILE:HG22	2.17	0.44
1:A:28:ARG:HH22	3:R:229:MET:CG	2.30	0.44
3:T:140:ILE:HG12	3:T:144:ALA:HB2	1.98	0.44
1:G:168:GLY:O	1:G:172:VAL:HG23	2.17	0.44
1:B:141:ILE:HD12	1:B:215:ILE:HG12	1.99	0.44
2:L:17:GLU:HB2	2:L:170:GLY:O	2.17	0.44
1:C:28:ARG:HH22	3:T:229:MET:HG3	1.82	0.44
2:K:187:LEU:HA	2:K:188:PRO:HD3	1.87	0.44
1:A:107:VAL:O	1:A:143:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:203:LEU:HD21	6:K:3097:HOH:O	2.17	0.44
2:K:196:ILE:HG23	2:K:201:LEU:HB2	1.98	0.44
2:I:17:GLU:HB2	2:I:170:GLY:O	2.18	0.44
1:C:109:ILE:HG13	1:C:142:ASP:HB3	1.98	0.44
2:H:163:LYS:NZ	2:H:171:GLY:O	2.51	0.44
2:H:171:GLY:H	2:H:203:LEU:HD13	1.82	0.44
3:T:86:GLU:OE2	3:T:121:GLU:OE2	2.35	0.44
1:D:152:ASP:HB2	1:D:153:PRO:CD	2.48	0.44
2:N:45:ILE:HB	2:N:52:ALA:HB1	1.99	0.44
1:E:109:ILE:HG13	1:E:142:ASP:HB3	1.99	0.44
3:O:140:ILE:HB	3:O:193:LYS:HB3	1.98	0.44
1:B:18:ASP:HB2	3:S:102:GLU:OE1	2.17	0.44
3:Q:89:ARG:CG	3:Q:117:ILE:HG21	2.48	0.44
3:T:140:ILE:HG22	3:T:197:ALA:HB2	1.99	0.44
1:D:141:ILE:HD13	1:D:146:PRO:HA	1.99	0.44
1:F:164:ALA:O	1:F:169:LYS:HG3	2.18	0.44
2:N:163:LYS:HZ1	2:N:203:LEU:HB3	1.81	0.44
1:E:61:GLN:HE21	1:E:62:ASN:H	1.62	0.44
2:I:18:ARG:HG3	2:I:172:MET:O	2.18	0.44
2:L:3:THR:HB	2:L:16:THR:HG22	2.00	0.44
2:K:18:ARG:CD	6:K:3054:HOH:O	2.65	0.44
2:H:13:ILE:HG12	2:H:177:VAL:HG22	1.99	0.44
2:L:131:SER:N	2:L:132:PRO:HD2	2.33	0.44
3:Q:101:GLU:HG3	3:R:105:LEU:HD22	2.00	0.43
2:J:74:MET:HG2	2:J:78:ALA:HB3	1.99	0.43
1:B:52:LYS:HB2	6:B:3033:HOH:O	2.18	0.43
1:A:71:ASP:HA	2:N:68:LEU:HD21	2.00	0.43
3:S:75:GLN:HG3	3:S:142:MET:O	2.18	0.43
2:M:172:MET:HE2	2:M:173:ILE:H	1.84	0.43
2:I:91:LYS:HD2	6:I:3093:HOH:O	2.16	0.43
3:T:82:TYR:OH	3:U:200:HIS:HB2	2.18	0.43
3:P:89:ARG:HD3	3:P:121:GLU:OE2	2.18	0.43
2:N:174:ASP:CG	6:N:3129:HOH:O	2.57	0.43
2:M:43:MET:HA	2:M:100:LEU:O	2.18	0.43
2:L:18:ARG:HB3	2:L:30:ASN:HA	2.00	0.43
2:I:157:ARG:HE	2:I:199:LEU:HD22	1.82	0.43
1:E:201:LEU:HA	1:E:201:LEU:HD12	1.79	0.43
3:R:117:ILE:O	3:R:121:GLU:HG3	2.18	0.43
3:O:64:PRO:HB2	3:O:67:LEU:HG	2.01	0.43
2:H:43:MET:HE3	2:H:56:VAL:HA	2.00	0.43
1:B:194:ILE:HD11	1:B:212:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TYR:HH	1:B:123:TYR:HH	1.67	0.43
3:Q:101:GLU:CG	3:R:105:LEU:HD22	2.49	0.43
1:C:122:GLN:HG3	6:C:3065:HOH:O	2.18	0.43
2:L:40:TYR:CD1	2:L:183:GLY:HA2	2.54	0.43
2:H:51:ASP:CG	2:I:91:LYS:HZ3	2.22	0.43
3:Q:155:VAL:HG12	3:Q:183:LEU:HD13	1.99	0.43
3:U:184:ARG:HG3	3:U:184:ARG:O	2.16	0.43
2:K:43:MET:CE	2:K:56:VAL:HG22	2.49	0.43
3:R:158:LYS:HB3	3:R:179:LEU:HD21	2.00	0.43
3:T:77:LEU:HG	3:T:77:LEU:O	2.19	0.43
2:L:59:MET:CE	2:L:79:VAL:HG13	2.48	0.43
3:S:136:ALA:HA	3:S:137:PRO:HD3	1.84	0.43
3:Q:28:TRP:HA	3:Q:32:THR:HB	2.01	0.43
1:D:12:ILE:HD13	1:D:131:PRO:HD3	1.99	0.42
1:G:55:ARG:O	1:G:56:SER:HB3	2.19	0.42
2:H:3:THR:HB	2:H:16:THR:HG22	2.01	0.42
2:M:40:TYR:HD1	2:M:183:GLY:HA2	1.83	0.42
1:E:81:LEU:HD23	3:U:230:VAL:HG23	2.00	0.42
1:F:175:PHE:CZ	1:F:195:LYS:HB3	2.54	0.42
1:A:17:PRO:HA	1:B:26:TYR:CD2	2.54	0.42
3:U:172:GLY:O	3:U:173:GLY:C	2.56	0.42
3:O:89:ARG:NH1	3:P:203:THR:HG21	2.34	0.42
3:O:63:SER:HA	3:O:64:PRO:HD3	1.87	0.42
1:E:12:ILE:HB	1:E:23:GLN:HG3	2.00	0.42
2:K:187:LEU:HB2	2:K:192:ILE:HD11	2.02	0.42
1:G:152:ASP:HB2	1:G:153:PRO:CD	2.50	0.42
1:B:52:LYS:HE2	1:B:52:LYS:HA	2.02	0.42
4:N:3021:SO4:O1	6:N:3128:HOH:O	2.21	0.42
1:D:185:PRO:HD2	1:D:188:GLU:HG3	2.02	0.42
1:G:225:ASP:OD1	1:G:227:GLU:HG3	2.18	0.42
3:R:184:ARG:NH1	3:R:184:ARG:CG	2.82	0.42
1:F:12:ILE:HG12	1:F:129:VAL:O	2.20	0.42
3:U:225:GLY:CA	6:U:290:HOH:O	2.67	0.42
2:L:157:ARG:HE	2:L:199:LEU:HD22	1.83	0.42
2:L:2:THR:OG1	2:L:130:GLY:HA3	2.19	0.42
1:F:97:GLN:OE1	1:F:97:GLN:HA	2.18	0.42
1:F:90:ASP:O	1:F:94:ILE:HG12	2.20	0.42
3:O:177:PRO:HG3	3:U:61:GLU:C	2.40	0.42
1:G:209:ALA:HA	1:G:210:PRO:HD2	1.95	0.42
1:A:143:GLN:CG	6:A:3017:HOH:O	2.67	0.42
1:B:158:ASN:HB2	1:B:160:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:116:ILE:O	3:R:204:MET:HE3	2.18	0.42
2:H:2:THR:OG1	2:H:130:GLY:HA3	2.19	0.42
1:B:13:THR:HB	1:C:130:ARG:HG2	2.00	0.42
3:R:221:GLN:CG	6:R:289:HOH:O	2.62	0.42
1:A:107:VAL:HG22	1:A:143:GLN:HE21	1.84	0.42
1:E:96:ALA:O	1:E:100:LYS:HG3	2.19	0.42
1:D:70:ILE:HG21	1:D:112:LEU:HD21	2.00	0.42
2:N:74:MET:HG2	2:N:78:ALA:HB3	2.01	0.42
3:S:63:SER:OG	3:T:181:LEU:HD12	2.19	0.42
2:N:195:ARG:HG2	2:N:198:LYS:HE3	2.02	0.42
1:G:76:ALA:HA	1:G:137:ILE:O	2.20	0.42
3:T:86:GLU:OE2	3:T:121:GLU:CD	2.58	0.42
1:A:67:ILE:HG12	1:A:77:VAL:HG13	2.00	0.42
3:O:62:LYS:HB2	3:O:62:LYS:HE3	1.77	0.42
3:S:77:LEU:HG	3:S:77:LEU:O	2.15	0.42
1:F:158:ASN:HB2	1:F:160:TYR:CE1	2.54	0.42
3:T:9:ILE:HD11	3:U:213:LEU:HB2	2.02	0.42
1:C:71:ASP:HA	2:I:68:LEU:HD21	2.01	0.42
1:C:139:ALA:HA	1:C:147:ARG:O	2.20	0.42
3:Q:87:THR:O	3:Q:91:VAL:HG23	2.20	0.42
3:O:89:ARG:HH12	3:P:203:THR:HG21	1.84	0.41
2:K:24:ASN:HB3	6:K:3095:HOH:O	2.19	0.41
2:L:57:ARG:HG3	5:L:2001:GOL:H2	2.01	0.41
1:E:172:VAL:HG13	1:E:196:ALA:HB1	2.02	0.41
1:D:64:ILE:HG22	1:D:64:ILE:O	2.20	0.41
1:D:175:PHE:HZ	1:D:195:LYS:HD3	1.85	0.41
1:C:62:ASN:HD22	1:C:62:ASN:H	1.67	0.41
2:K:172:MET:CE	2:K:192:ILE:CG2	2.98	0.41
3:Q:56:GLY:H	3:Q:59:GLN:HE21	1.67	0.41
3:O:138:THR:HA	3:O:139:PRO:HD3	1.97	0.41
3:Q:130:LYS:O	3:R:136:ALA:N	2.43	0.41
3:U:36:ILE:HG13	3:U:77:LEU:HD11	2.02	0.41
1:B:52:LYS:CB	6:B:3033:HOH:O	2.67	0.41
1:E:12:ILE:HA	1:E:23:GLN:CG	2.49	0.41
3:T:75:GLN:HG3	3:T:142:MET:O	2.20	0.41
3:T:56:GLY:H	3:T:59:GLN:NE2	2.18	0.41
2:J:172:MET:HE3	6:J:3093:HOH:O	2.19	0.41
2:N:43:MET:HB3	2:N:43:MET:HE2	1.96	0.41
3:T:101:GLU:HG3	3:U:105:LEU:HD22	2.02	0.41
1:D:107:VAL:HG13	1:D:143:GLN:HG2	2.02	0.41
1:D:110:GLU:CD	6:D:3051:HOH:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:149:LEU:O	3:U:153:SER:HB2	2.20	0.41
2:K:113:ILE:HA	2:K:118:GLY:O	2.20	0.41
3:O:152:ARG:NH1	3:O:156:GLU:OE2	2.50	0.41
2:N:113:ILE:HA	2:N:118:GLY:O	2.21	0.41
2:L:113:ILE:HA	2:L:118:GLY:O	2.20	0.41
1:C:12:ILE:HD13	1:C:131:PRO:HD3	2.03	0.41
2:J:163:LYS:NZ	2:J:203:LEU:HB3	2.36	0.41
1:E:201:LEU:O	1:E:205:GLU:OE1	2.39	0.41
1:A:66:LYS:HE2	1:A:78:THR:H	1.86	0.41
2:M:141:GLN:OE1	2:M:157:ARG:NH2	2.53	0.41
1:D:83:ALA:HB3	6:D:3009:HOH:O	2.20	0.41
1:E:173:VAL:O	1:E:177:GLU:HG3	2.20	0.41
2:M:58[A]:TYR:CE2	2:M:59:MET:CE	3.03	0.41
1:F:160:TYR:CE2	1:G:59:ILE:HD13	2.56	0.41
1:C:17:PRO:HB3	3:U:105:LEU:HD11	2.03	0.41
3:Q:116:ILE:HG12	3:Q:208:VAL:HG22	2.02	0.41
2:M:24:ASN:ND2	2:M:24:ASN:H	2.18	0.41
2:K:157:ARG:CD	6:K:3051:HOH:O	2.67	0.41
3:S:159:LEU:O	3:S:173:GLY:HA3	2.21	0.41
1:C:175:PHE:CZ	1:C:179:GLU:HG3	2.56	0.41
3:S:202:SER:O	3:S:206:ARG:HG3	2.20	0.41
2:H:172:MET:HE2	2:H:189:THR:HG23	2.02	0.41
2:H:19:ARG:HD3	2:H:26:ILE:HG12	2.03	0.41
3:U:9:ILE:O	3:U:12:LEU:HB2	2.21	0.41
2:K:143:SER:HB3	2:K:146:MET:HG3	2.01	0.41
3:T:140:ILE:HB	3:T:193:LYS:HB3	2.03	0.41
3:R:159:LEU:O	3:R:173:GLY:HA3	2.20	0.41
3:U:90:THR:O	3:U:94:ILE:HG12	2.21	0.41
1:A:69:LEU:HD23	1:A:75:ALA:HB2	2.03	0.41
3:P:51:ARG:O	3:P:184:ARG:NH2	2.54	0.41
3:P:146:ARG:HD3	6:P:259:HOH:O	2.20	0.41
1:D:73:TYR:O	1:D:140:GLY:HA3	2.20	0.41
1:A:187:LYS:HE3	1:A:231:LYS:HZ3	1.84	0.41
2:N:172:MET:HE3	2:N:173:ILE:N	2.33	0.41
1:E:107:VAL:O	1:E:142:ASP:HB2	2.21	0.41
1:E:12:ILE:HA	1:E:23:GLN:HG3	2.03	0.41
3:P:101:GLU:HG3	3:Q:105:LEU:CD2	2.51	0.41
2:M:172:MET:CE	2:M:173:ILE:H	2.34	0.40
1:A:143:GLN:HB3	6:A:3017:HOH:O	2.20	0.40
3:P:89:ARG:HH11	3:P:89:ARG:HD2	1.75	0.40
3:R:191:MET:O	3:R:195:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:GLN:OE1	1:E:97:GLN:HA	2.21	0.40
2:N:202:ILE:CG1	2:N:203:LEU:N	2.82	0.40
2:N:202:ILE:CD1	2:N:203:LEU:H	2.34	0.40
1:D:54:VAL:HG13	1:D:61:GLN:NE2	2.37	0.40
3:S:89:ARG:HD3	3:S:117:ILE:HG22	2.03	0.40
3:R:10:GLN:NE2	3:R:14:ASP:OD1	2.48	0.40
2:K:32:LYS:HE2	6:K:3092:HOH:O	2.21	0.40
1:E:208:LYS:N	1:E:208:LYS:CD	2.55	0.40
2:J:172:MET:CE	2:J:173:ILE:H	2.34	0.40
3:S:24:VAL:HG13	3:S:84:GLN:HB3	2.04	0.40
3:T:39:ILE:HD13	3:T:74:TYR:HA	2.03	0.40
1:G:13:THR:HG21	1:G:126:TYR:C	2.42	0.40
3:U:140:ILE:CD1	3:U:144:ALA:HB1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	220/233 (94%)	208 (94%)	6 (3%)	6 (3%)	6 6
1	B	220/233 (94%)	204 (93%)	13 (6%)	3 (1%)	14 19
1	C	220/233 (94%)	211 (96%)	5 (2%)	4 (2%)	11 13
1	D	220/233 (94%)	202 (92%)	16 (7%)	2 (1%)	21 30
1	E	220/233 (94%)	210 (96%)	8 (4%)	2 (1%)	21 30
1	F	220/233 (94%)	206 (94%)	11 (5%)	3 (1%)	14 19
1	G	220/233 (94%)	205 (93%)	10 (4%)	5 (2%)	8 8
2	H	203/217 (94%)	195 (96%)	8 (4%)	0	100 100
2	I	203/217 (94%)	196 (97%)	7 (3%)	0	100 100
2	J	203/217 (94%)	194 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	202/217 (93%)	196 (97%)	6 (3%)	0	100	100
2	L	202/217 (93%)	197 (98%)	4 (2%)	1 (0%)	34	48
2	M	203/217 (94%)	196 (97%)	7 (3%)	0	100	100
2	N	203/217 (94%)	195 (96%)	7 (3%)	1 (0%)	34	48
3	O	214/237 (90%)	208 (97%)	6 (3%)	0	100	100
3	P	214/237 (90%)	209 (98%)	4 (2%)	1 (0%)	34	48
3	Q	214/237 (90%)	206 (96%)	8 (4%)	0	100	100
3	R	214/237 (90%)	206 (96%)	8 (4%)	0	100	100
3	S	214/237 (90%)	206 (96%)	8 (4%)	0	100	100
3	T	214/237 (90%)	208 (97%)	6 (3%)	0	100	100
3	U	214/237 (90%)	208 (97%)	5 (2%)	1 (0%)	34	48
All	All	4457/4809 (93%)	4266 (96%)	162 (4%)	29 (1%)	26	38

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	C	62	ASN
1	C	209	ALA
1	D	54	VAL
1	D	56	SER
1	F	56	SER
1	F	202	GLU
1	G	182	GLU
1	A	62	ASN
1	B	231	LYS
1	E	202	GLU
1	E	203	GLU
1	G	56	SER
2	N	202	ILE
3	U	173	GLY
1	A	55	ARG
1	B	62	ASN
1	G	65	GLU
3	P	226	SER
1	B	56	SER
1	A	109	ILE
1	C	231	LYS

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Mol	Chain	Res	Type
1	A	67	ILE
2	L	202	ILE
1	A	64	ILE
1	G	209	ALA
1	F	64	ILE
1	G	64	ILE
1	C	64	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	185/191 (97%)	165 (89%)	20 (11%)	8 11
1	B	185/191 (97%)	172 (93%)	13 (7%)	19 29
1	C	185/191 (97%)	174 (94%)	11 (6%)	24 38
1	D	185/191 (97%)	171 (92%)	14 (8%)	16 25
1	E	185/191 (97%)	173 (94%)	12 (6%)	21 33
1	F	185/191 (97%)	176 (95%)	9 (5%)	31 48
1	G	185/191 (97%)	174 (94%)	11 (6%)	24 38
2	H	172/183 (94%)	160 (93%)	12 (7%)	19 29
2	I	172/183 (94%)	158 (92%)	14 (8%)	15 22
2	J	172/183 (94%)	152 (88%)	20 (12%)	7 9
2	K	171/183 (93%)	160 (94%)	11 (6%)	22 34
2	L	171/183 (93%)	154 (90%)	17 (10%)	10 14
2	M	172/183 (94%)	163 (95%)	9 (5%)	29 45
2	N	172/183 (94%)	159 (92%)	13 (8%)	16 25
3	O	179/196 (91%)	171 (96%)	8 (4%)	34 52
3	P	179/196 (91%)	174 (97%)	5 (3%)	51 72
3	Q	179/196 (91%)	171 (96%)	8 (4%)	34 52
3	R	179/196 (91%)	170 (95%)	9 (5%)	30 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	S	179/196 (91%)	176 (98%)	3 (2%)	68 85
3	T	179/196 (91%)	171 (96%)	8 (4%)	34 52
3	U	179/196 (91%)	175 (98%)	4 (2%)	60 79
All	All	3750/3990 (94%)	3519 (94%)	231 (6%)	23 35

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	14	VAL
1	A	35	SER
1	A	52	LYS
1	A	53	LYS
1	A	56	SER
1	A	61	GLN
1	A	64	ILE
1	A	65	GLU
1	A	66	LYS
1	A	77	VAL
1	A	106	LEU
1	A	129	VAL
1	A	152	ASP
1	A	157	ILE
1	A	177	GLU
1	A	181	LYS
1	A	202	GLU
1	A	226	GLN
1	A	230	LYS
1	B	12	ILE
1	B	14	VAL
1	B	52	LYS
1	B	53	LYS
1	B	61	GLN
1	B	62	ASN
1	B	65	GLU
1	B	88	LEU
1	B	129	VAL
1	B	135	SER
1	B	201	LEU
1	B	202	GLU
1	B	221	TYR

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Mol	Chain	Res	Type
1	C	12	ILE
1	C	59	ILE
1	C	61	GLN
1	C	62	ASN
1	C	63	SER
1	C	177	GLU
1	C	202	GLU
1	C	208	LYS
1	C	221	TYR
1	C	222	ARG
1	C	230	LYS
1	D	12	ILE
1	D	65	GLU
1	D	143	GLN
1	D	157	ILE
1	D	174	SER
1	D	181	LYS
1	D	182	GLU
1	D	187	LYS
1	D	203	GLU
1	D	212	ILE
1	D	221	TYR
1	D	226	GLN
1	D	227	GLU
1	D	233	LEU
1	E	12	ILE
1	E	14	VAL
1	E	35	SER
1	E	55	ARG
1	E	61	GLN
1	E	63	SER
1	E	64	ILE
1	E	66	LYS
1	E	106	LEU
1	E	153	PRO
1	E	201	LEU
1	E	208	LYS
1	F	12	ILE
1	F	53	LYS
1	F	55	ARG
1	F	62	ASN
1	F	202	GLU

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Mol	Chain	Res	Type
1	F	203	GLU
1	F	221	TYR
1	F	225	ASP
1	F	227	GLU
1	G	12	ILE
1	G	14	VAL
1	G	44	ASN
1	G	54	VAL
1	G	135	SER
1	G	176	LEU
1	G	202	GLU
1	G	221	TYR
1	G	225	ASP
1	G	226	GLN
1	G	230	LYS
2	H	3	THR
2	H	17	GLU
2	H	23	GLU
2	H	25	PHE
2	H	30	ASN
2	H	68	LEU
2	H	91	LYS
2	H	105	ASP
2	H	112	SER
2	H	174	ASP
2	H	190	ASP
2	H	203	LEU
2	I	9	LYS
2	I	17	GLU
2	I	23	GLU
2	I	25	PHE
2	I	68	LEU
2	I	84	SER
2	I	104	ILE
2	I	105	ASP
2	I	112	SER
2	I	144	GLU
2	I	174	ASP
2	I	185	VAL
2	I	202	ILE
2	I	203	LEU
2	J	3	THR

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Mol	Chain	Res	Type
2	J	9	LYS
2	J	17	GLU
2	J	18	ARG
2	J	22	MET
2	J	23	GLU
2	J	24	ASN
2	J	25	PHE
2	J	68	LEU
2	J	71	ARG
2	J	105	ASP
2	J	123	ILE
2	J	144	GLU
2	J	174	ASP
2	J	186	GLN
2	J	190	ASP
2	J	194	SER
2	J	197	ARG
2	J	202	ILE
2	J	203	LEU
2	K	3	THR
2	K	17	GLU
2	K	25	PHE
2	K	27	MET
2	K	68	LEU
2	K	84	SER
2	K	105	ASP
2	K	144	GLU
2	K	181	LYS
2	K	186	GLN
2	K	203	LEU
2	L	3	THR
2	L	9	LYS
2	L	17	GLU
2	L	24	ASN
2	L	25	PHE
2	L	27	MET
2	L	30	ASN
2	L	68	LEU
2	L	91	LYS
2	L	123	ILE
2	L	174	ASP
2	L	180	ARG

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Mol	Chain	Res	Type
2	L	189	THR
2	L	194	SER
2	L	201	LEU
2	L	202	ILE
2	L	203	LEU
2	M	17	GLU
2	M	22	MET
2	M	25	PHE
2	M	91	LYS
2	M	113	ILE
2	M	172	MET
2	M	174	ASP
2	M	198	LYS
2	M	202	ILE
2	N	9	LYS
2	N	17	GLU
2	N	23	GLU
2	N	24	ASN
2	N	25	PHE
2	N	30	ASN
2	N	68	LEU
2	N	96[A]	MET
2	N	96[B]	MET
2	N	172	MET
2	N	174	ASP
2	N	194	SER
2	N	202	ILE
3	O	15	SER
3	O	53	SER
3	O	89	ARG
3	O	119	GLU
3	O	129	GLU
3	O	146	ARG
3	O	157	ASP
3	O	224	THR
3	P	115	LYS
3	P	131	SER
3	P	140	ILE
3	P	153	SER
3	P	219	LEU
3	Q	10	GLN
3	Q	52	ASN

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Mol	Chain	Res	Type
3	Q	53	SER
3	Q	145	LEU
3	Q	157	ASP
3	Q	221	GLN
3	Q	227	ASP
3	Q	231	SER
3	R	61	GLU
3	R	62	LYS
3	R	63	SER
3	R	77	LEU
3	R	115	LYS
3	R	123	LYS
3	R	150	SER
3	R	153	SER
3	R	184	ARG
3	S	4	LYS
3	S	77	LEU
3	S	224	THR
3	T	4	LYS
3	T	10	GLN
3	T	37	GLU
3	T	52	ASN
3	T	63	SER
3	T	77	LEU
3	T	224	THR
3	T	226	SER
3	U	63	SER
3	U	77	LEU
3	U	184	ARG
3	U	224	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	B	62	ASN
1	B	183	ASN
1	C	62	ASN
1	C	226	GLN
1	D	61	GLN
1	D	62	ASN
1	D	226	GLN

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Mol	Chain	Res	Type
1	E	61	GLN
1	E	62	ASN
1	E	226	GLN
1	F	62	ASN
1	F	226	GLN
1	G	122	GLN
2	H	24	ASN
2	I	24	ASN
2	I	186	GLN
2	I	191	GLN
2	J	24	ASN
2	J	30	ASN
2	J	186	GLN
2	J	191	GLN
2	K	24	ASN
2	L	24	ASN
2	L	191	GLN
2	M	24	ASN
2	N	24	ASN
2	N	186	GLN
2	N	191	GLN
3	O	52	ASN
3	O	79	HIS
3	P	79	HIS
3	Q	59	GLN
3	Q	79	HIS
3	R	59	GLN
3	R	79	HIS
3	R	99	HIS
3	S	47	HIS
3	S	99	HIS
3	T	59	GLN
3	T	79	HIS
3	T	99	HIS
3	T	221	GLN
3	U	79	HIS
3	U	175	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	3007	-	4,4,4	0.19	0	6,6,6	0.24	0
4	SO4	B	3001	-	4,4,4	0.20	0	6,6,6	0.12	0
4	SO4	C	3002	-	4,4,4	0.17	0	6,6,6	0.12	0
4	SO4	D	3003	-	4,4,4	0.18	0	6,6,6	0.22	0
4	SO4	E	3004	-	4,4,4	0.10	0	6,6,6	0.24	0
4	SO4	F	3005	-	4,4,4	0.36	0	6,6,6	0.14	0
4	SO4	G	3006	-	4,4,4	0.19	0	6,6,6	0.15	0
5	GOL	H	2004	-	5,5,5	0.41	0	5,5,5	1.01	0
4	SO4	H	3008	-	4,4,4	0.51	0	6,6,6	0.66	0
4	SO4	H	3015	-	4,4,4	0.32	0	6,6,6	0.63	0
5	GOL	I	2005	-	5,5,5	0.32	0	5,5,5	0.73	0
4	SO4	I	3011	-	4,4,4	0.40	0	6,6,6	0.50	0
4	SO4	I	3016	-	4,4,4	0.21	0	6,6,6	0.83	0
4	SO4	I	3023	-	4,4,4	0.25	0	6,6,6	0.24	0
5	GOL	J	2006	-	5,5,5	0.47	0	5,5,5	0.34	0
4	SO4	J	3012	-	4,4,4	0.24	0	6,6,6	0.28	0
4	SO4	J	3017	-	4,4,4	0.43	0	6,6,6	0.31	0
5	GOL	K	2007	-	5,5,5	0.79	0	5,5,5	1.21	1 (20%)
4	SO4	K	3013	-	4,4,4	0.32	0	6,6,6	0.53	0
4	SO4	K	3018	-	4,4,4	0.21	0	6,6,6	0.56	0
5	GOL	L	2001	-	5,5,5	0.36	0	5,5,5	0.65	0
4	SO4	L	3014	-	4,4,4	0.28	0	6,6,6	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	L	3019	-	4,4,4	0.34	0	6,6,6	0.85	1 (16%)
5	GOL	M	2002	-	5,5,5	0.55	0	5,5,5	0.87	0
4	SO4	M	3010	-	4,4,4	0.19	0	6,6,6	0.44	0
4	SO4	M	3020	-	4,4,4	0.21	0	6,6,6	0.66	0
4	SO4	M	3024	-	4,4,4	0.16	0	6,6,6	0.22	0
4	SO4	M	3025	-	4,4,4	0.20	0	6,6,6	0.40	0
5	GOL	N	2003	-	5,5,5	0.31	0	5,5,5	0.42	0
4	SO4	N	3009	-	4,4,4	0.26	0	6,6,6	0.38	0
4	SO4	N	3021	-	4,4,4	0.29	0	6,6,6	0.42	0
4	SO4	N	3022	-	4,4,4	0.13	0	6,6,6	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	3007	-	-	0/0/0/0	0/0/0/0
4	SO4	B	3001	-	-	0/0/0/0	0/0/0/0
4	SO4	C	3002	-	-	0/0/0/0	0/0/0/0
4	SO4	D	3003	-	-	0/0/0/0	0/0/0/0
4	SO4	E	3004	-	-	0/0/0/0	0/0/0/0
4	SO4	F	3005	-	-	0/0/0/0	0/0/0/0
4	SO4	G	3006	-	-	0/0/0/0	0/0/0/0
5	GOL	H	2004	-	-	0/4/4/4	0/0/0/0
4	SO4	H	3008	-	-	0/0/0/0	0/0/0/0
4	SO4	H	3015	-	-	0/0/0/0	0/0/0/0
5	GOL	I	2005	-	-	0/4/4/4	0/0/0/0
4	SO4	I	3011	-	-	0/0/0/0	0/0/0/0
4	SO4	I	3016	-	-	0/0/0/0	0/0/0/0
4	SO4	I	3023	-	-	0/0/0/0	0/0/0/0
5	GOL	J	2006	-	-	0/4/4/4	0/0/0/0
4	SO4	J	3012	-	-	0/0/0/0	0/0/0/0
4	SO4	J	3017	-	-	0/0/0/0	0/0/0/0
5	GOL	K	2007	-	-	0/4/4/4	0/0/0/0
4	SO4	K	3013	-	-	0/0/0/0	0/0/0/0
4	SO4	K	3018	-	-	0/0/0/0	0/0/0/0
5	GOL	L	2001	-	-	0/4/4/4	0/0/0/0
4	SO4	L	3014	-	-	0/0/0/0	0/0/0/0
4	SO4	L	3019	-	-	0/0/0/0	0/0/0/0
5	GOL	M	2002	-	-	0/4/4/4	0/0/0/0
4	SO4	M	3010	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	M	3020	-	-	0/0/0/0	0/0/0/0
4	SO4	M	3024	-	-	0/0/0/0	0/0/0/0
4	SO4	M	3025	-	-	0/0/0/0	0/0/0/0
5	GOL	N	2003	-	-	0/4/4/4	0/0/0/0
4	SO4	N	3009	-	-	0/0/0/0	0/0/0/0
4	SO4	N	3021	-	-	0/0/0/0	0/0/0/0
4	SO4	N	3022	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	2007	GOL	O3-C3-C2	-2.08	100.10	110.18
4	L	3019	SO4	O2-S-O1	-2.02	103.11	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3007	SO4	2	0
4	D	3003	SO4	1	0
4	I	3016	SO4	1	0
4	J	3017	SO4	1	0
5	L	2001	GOL	2	0
4	L	3019	SO4	1	0
4	M	3010	SO4	1	0
4	N	3021	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	222/233 (95%)	-0.21	19 (8%)	13	13	21, 36, 77, 85	0
1	B	222/233 (95%)	-0.21	17 (7%)	16	16	21, 36, 72, 86	0
1	C	222/233 (95%)	-0.21	20 (9%)	12	11	21, 36, 73, 86	0
1	D	222/233 (95%)	-0.12	18 (8%)	15	14	23, 39, 76, 87	0
1	E	222/233 (95%)	-0.30	13 (5%)	26	26	23, 35, 66, 78	0
1	F	222/233 (95%)	-0.11	19 (8%)	13	13	24, 39, 77, 88	0
1	G	222/233 (95%)	-0.05	22 (9%)	9	9	24, 38, 75, 88	0
2	H	203/217 (93%)	-0.69	3 (1%)	76	75	20, 28, 48, 78	0
2	I	203/217 (93%)	-0.65	4 (1%)	68	68	21, 29, 50, 71	0
2	J	203/217 (93%)	-0.62	3 (1%)	76	75	22, 30, 51, 76	0
2	K	203/217 (93%)	-0.65	7 (3%)	49	49	22, 30, 51, 74	0
2	L	203/217 (93%)	-0.59	5 (2%)	61	60	22, 30, 50, 73	0
2	M	203/217 (93%)	-0.70	3 (1%)	76	75	21, 29, 46, 69	0
2	N	203/217 (93%)	-0.69	2 (0%)	84	83	20, 29, 49, 71	0
3	O	218/237 (91%)	0.05	17 (7%)	16	15	30, 46, 72, 80	0
3	P	218/237 (91%)	0.14	13 (5%)	25	25	32, 49, 77, 86	0
3	Q	218/237 (91%)	0.18	17 (7%)	16	15	30, 50, 76, 93	0
3	R	218/237 (91%)	0.03	16 (7%)	18	18	25, 44, 76, 85	0
3	S	218/237 (91%)	-0.24	13 (5%)	25	25	23, 37, 72, 85	0
3	T	218/237 (91%)	-0.19	13 (5%)	25	25	24, 38, 69, 84	0
3	U	218/237 (91%)	-0.16	15 (6%)	20	19	25, 38, 73, 87	0
All	All	4501/4809 (93%)	-0.28	259 (5%)	26	27	20, 36, 72, 93	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	225	GLY	10.4
3	Q	227	ASP	9.2
1	G	204	GLY	8.9
2	L	203	LEU	8.8
3	U	225	GLY	8.7
2	I	203	LEU	8.7
2	H	203	LEU	8.0
1	B	64	ILE	7.8
3	U	226	SER	7.7
3	R	226	SER	7.5
3	P	226	SER	7.4
3	R	225	GLY	7.3
1	A	62	ASN	7.1
3	S	228	HIS	7.1
2	H	202	ILE	7.1
3	T	228	HIS	7.0
3	O	226	SER	7.0
3	R	172	GLY	6.9
3	T	225	GLY	6.9
2	N	203	LEU	6.7
3	S	226	SER	6.7
3	P	225	GLY	6.6
1	C	64	ILE	6.6
1	D	64	ILE	6.6
2	J	203	LEU	6.5
3	O	131	SER	6.5
1	G	64	ILE	6.5
3	Q	225	GLY	6.5
3	P	228	HIS	6.4
3	T	226	SER	6.4
3	S	225	GLY	6.3
3	T	131	SER	6.2
1	D	12	ILE	6.1
2	M	203	LEU	6.1
3	Q	226	SER	6.0
3	Q	228	HIS	6.0
2	K	203	LEU	6.0
3	R	228	HIS	5.9
1	F	55	ARG	5.8
3	P	227	ASP	5.6
1	B	204	GLY	5.5
3	U	228	HIS	5.5
1	B	12	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	F	64	ILE	5.5
1	G	233	LEU	5.4
3	Q	172	GLY	5.3
3	Q	131	SER	5.3
1	G	55	ARG	5.3
3	U	227	ASP	5.3
1	E	55	ARG	5.3
1	G	12	ILE	5.3
3	R	133	SER	5.2
1	D	13	THR	5.1
1	A	55	ARG	5.1
3	O	228	HIS	5.1
1	F	13	THR	5.0
1	D	62	ASN	5.0
3	T	134	GLY	4.9
3	O	227	ASP	4.8
3	Q	231	SER	4.8
3	T	172	GLY	4.8
1	A	206	GLU	4.7
1	F	202	GLU	4.6
3	S	133	SER	4.6
3	R	227	ASP	4.6
3	U	131	SER	4.5
1	F	62	ASN	4.5
3	S	172	GLY	4.4
3	U	134	GLY	4.4
1	G	174	SER	4.3
3	Q	230	VAL	4.3
1	C	227	GLU	4.3
3	S	131	SER	4.3
1	A	204	GLY	4.3
1	F	53	LYS	4.3
3	T	133	SER	4.3
2	L	202	ILE	4.2
1	A	203	GLU	4.2
1	E	202	GLU	4.2
1	D	55	ARG	4.2
3	R	131	SER	4.2
1	A	65	GLU	4.2
1	E	12	ILE	4.1
3	Q	52	ASN	4.1
1	E	64	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	206	GLU	4.0
1	G	202	GLU	4.0
3	P	131	SER	4.0
3	T	227	ASP	4.0
3	P	52	ASN	4.0
3	O	134	GLY	3.9
1	C	13	THR	3.9
1	C	204	GLY	3.9
1	F	203	GLU	3.9
1	E	54	VAL	3.9
1	B	174	SER	3.9
3	S	227	ASP	3.9
3	R	48	GLY	3.9
3	P	132	GLY	3.8
1	F	227	GLU	3.8
2	N	202	ILE	3.7
1	A	202	GLU	3.7
1	A	226	GLN	3.7
1	C	54	VAL	3.7
2	M	202	ILE	3.6
1	F	226	GLN	3.6
1	C	206	GLU	3.6
1	F	233	LEU	3.6
1	A	13	THR	3.6
1	C	53	LYS	3.6
1	E	204	GLY	3.6
3	R	132	GLY	3.6
1	C	55	ARG	3.6
2	J	202	ILE	3.5
1	G	203	GLU	3.5
1	D	208	LYS	3.5
1	D	63	SER	3.5
1	C	62	ASN	3.5
1	G	227	GLU	3.4
1	C	208	LYS	3.4
1	F	12	ILE	3.4
1	C	203	GLU	3.4
1	G	206	GLU	3.4
2	I	202	ILE	3.4
1	B	203	GLU	3.3
1	B	202	GLU	3.3
1	E	203	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	K	202	ILE	3.3
1	G	62	ASN	3.3
3	O	172	GLY	3.3
1	D	54	VAL	3.3
3	O	52	ASN	3.3
1	A	225	ASP	3.3
1	B	226	GLN	3.3
3	R	161	GLY	3.2
1	G	63	SER	3.2
1	B	227	GLU	3.2
1	G	13	THR	3.2
1	G	205	GLU	3.2
1	C	61	GLN	3.2
1	D	206	GLU	3.2
1	F	205	GLU	3.2
1	B	55	ARG	3.2
1	F	206	GLU	3.2
3	P	134	GLY	3.1
1	E	62	ASN	3.1
1	C	12	ILE	3.1
1	G	53	LYS	3.1
1	C	202	GLU	3.1
1	E	226	GLN	3.1
3	P	133	SER	3.1
1	D	204	GLY	3.1
3	U	137	PRO	3.0
1	G	208	LYS	3.0
1	D	209	ALA	3.0
3	O	133	SER	3.0
3	O	58	ALA	3.0
1	A	61	GLN	3.0
1	C	233	LEU	3.0
3	U	231	SER	3.0
1	G	54	VAL	2.9
1	C	231	LYS	2.9
1	G	61	GLN	2.9
3	P	10	GLN	2.9
1	B	54	VAL	2.9
1	A	233	LEU	2.9
1	B	13	THR	2.9
1	G	181	LYS	2.9
1	F	201	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	13	THR	2.9
1	A	187	LYS	2.8
3	R	134	GLY	2.8
1	F	204	GLY	2.8
1	F	61	GLN	2.8
1	E	227	GLU	2.8
1	A	227	GLU	2.8
2	J	22	MET	2.8
1	F	225	ASP	2.8
2	I	200	GLY	2.8
1	E	53	LYS	2.7
1	D	227	GLU	2.7
3	R	231	SER	2.7
1	A	53	LYS	2.7
3	Q	173	GLY	2.7
1	D	53	LYS	2.7
3	Q	133	SER	2.7
1	A	205	GLU	2.7
3	T	224	THR	2.6
1	A	12	ILE	2.6
2	L	22	MET	2.6
3	U	161	GLY	2.6
1	F	174	SER	2.6
3	S	128	GLY	2.6
3	T	54	THR	2.6
3	S	132	GLY	2.5
1	B	62	ASN	2.5
1	B	205	GLU	2.5
1	D	174	SER	2.5
1	G	187	LYS	2.5
1	D	203	GLU	2.5
3	U	135	GLY	2.5
3	Q	132	GLY	2.5
3	Q	129	GLU	2.5
1	D	202	GLU	2.4
3	O	173	GLY	2.4
2	M	22	MET	2.4
3	P	161	GLY	2.4
3	S	134	GLY	2.4
1	D	225	ASP	2.4
3	T	130	LYS	2.3
2	K	149	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	22	MET	2.3
3	P	53	SER	2.3
3	R	52	ASN	2.3
3	S	224	THR	2.3
1	D	226	GLN	2.3
1	B	208	LYS	2.3
3	U	129	GLU	2.3
1	C	44	ASN	2.3
3	T	230	VAL	2.3
1	G	191	THR	2.2
1	A	63	SER	2.2
3	R	230	VAL	2.2
3	U	136	ALA	2.2
3	U	132	GLY	2.2
2	K	181	LYS	2.2
1	C	225	ASP	2.2
2	K	194	SER	2.2
2	L	181	LYS	2.2
1	C	205	GLU	2.2
3	S	230	VAL	2.2
3	O	11	ASN	2.2
1	B	53	LYS	2.2
2	L	200	GLY	2.2
3	O	10	GLN	2.2
3	R	173	GLY	2.2
3	Q	45	GLU	2.1
3	S	137	PRO	2.1
1	C	226	GLN	2.1
1	F	208	LYS	2.1
3	O	161	GLY	2.1
2	H	22	MET	2.1
3	O	65	GLU	2.1
2	I	22	MET	2.1
1	G	143	GLN	2.1
3	Q	134	GLY	2.1
3	Q	175	GLN	2.1
3	R	175	GLN	2.1
3	P	65	GLU	2.1
3	Q	48	GLY	2.1
3	O	53	SER	2.1
3	U	10	GLN	2.0
1	A	66	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	225	ASP	2.0
3	U	133	SER	2.0
2	K	190	ASP	2.0
3	O	45	GLU	2.0
1	E	63	SER	2.0
3	T	52	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	H	3015	5/5	0.96	0.16	12.67	47,49,51,51	0
4	SO4	N	3009	5/5	0.98	0.16	6.98	46,47,50,50	0
4	SO4	L	3014	5/5	0.98	0.18	5.81	46,47,50,51	0
4	SO4	M	3010	5/5	0.98	0.18	5.57	50,53,55,55	0
4	SO4	H	3008	5/5	0.97	0.17	5.24	47,47,50,52	0
4	SO4	M	3025	5/5	0.94	0.26	3.65	77,77,79,79	0
4	SO4	N	3022	5/5	0.93	0.15	3.16	89,90,91,91	0
4	SO4	K	3018	5/5	0.97	0.16	2.99	56,57,57,57	0
4	SO4	I	3023	5/5	0.91	0.15	2.90	83,83,84,84	0
4	SO4	I	3011	5/5	0.98	0.10	2.71	38,40,43,46	0
4	SO4	K	3013	5/5	0.98	0.15	2.25	42,43,47,49	0
4	SO4	I	3016	5/5	0.97	0.13	2.07	51,52,56,56	0
4	SO4	L	3019	5/5	0.97	0.13	1.88	56,58,58,59	0
4	SO4	M	3020	5/5	0.97	0.15	1.84	63,64,64,65	0
4	SO4	M	3024	5/5	0.93	0.14	1.77	82,84,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	E	3004	5/5	0.78	0.36	1.45	120,121,121,121	0
4	SO4	J	3012	5/5	0.98	0.13	1.40	44,44,47,48	0
4	SO4	N	3021	5/5	0.97	0.12	1.07	54,55,58,59	0
5	GOL	L	2001	6/6	0.95	0.11	0.70	41,41,42,44	0
4	SO4	J	3017	5/5	0.98	0.11	0.70	49,50,50,52	0
4	SO4	F	3005	5/5	0.83	0.30	0.69	112,112,113,113	0
5	GOL	M	2002	6/6	0.96	0.09	0.68	49,51,52,52	0
5	GOL	J	2006	6/6	0.94	0.10	0.55	37,41,46,50	0
5	GOL	K	2007	6/6	0.94	0.11	0.54	38,39,41,42	0
5	GOL	I	2005	6/6	0.98	0.09	0.19	36,38,41,44	0
4	SO4	B	3001	5/5	0.84	0.25	0.18	128,128,128,128	0
4	SO4	A	3007	5/5	0.81	0.30	0.07	116,117,117,117	0
5	GOL	H	2004	6/6	0.95	0.10	-0.12	42,42,44,44	0
4	SO4	G	3006	5/5	0.90	0.21	-0.23	114,114,114,114	0
4	SO4	D	3003	5/5	0.91	0.20	-0.26	105,105,105,106	0
4	SO4	C	3002	5/5	0.93	0.20	-0.30	110,110,110,110	0
5	GOL	N	2003	6/6	0.97	0.08	-0.39	44,45,46,46	0

6.5 Other polymers

There are no such residues in this entry.